

data\_jgb Λ-(S,S)-3<sup>3+</sup> 3Cl<sup>-</sup>

\_audit\_creation\_method                    SHELXL-97  
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;  
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\_chemical\_formula\_weight                902.26

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'C' 'C' 0.0033 0.0016  
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
'H' 'H' 0.0000 0.0000  
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
'Cl' 'Cl' 0.1484 0.1585  
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
'Co' 'Co' 0.3494 0.9721  
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
'N' 'N' 0.0061 0.0033  
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
'O' 'O' 0.0106 0.0060  
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

\_symmetry\_cell\_setting                Tetragonal  
\_symmetry\_space\_group\_name\_H-M      P4(3)

loop\_  
\_symmetry\_equiv\_pos\_as\_xyz  
'x, y, z'  
'-x, -y, z+1/2'  
'-y, x, z+3/4'  
'y, -x, z+1/4'

\_cell\_length\_a                        13.839(4)  
\_cell\_length\_b                        13.839(4)  
\_cell\_length\_c                        24.216(9)

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\_cell\_angle\_beta 90.00  
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\_cell\_volume 4638(2)  
\_cell\_formula\_units\_Z 4  
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\_exptl\_crystal\_description block  
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\_exptl\_crystal\_density\_diffrn 1.292  
\_exptl\_crystal\_density\_method 'not measured'  
\_exptl\_crystal\_F\_000 1904  
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\_diffrn\_ambient\_temperature 110(2)  
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\_diffrn\_measurement\_method 'omega scans'  
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APEX-II(BRUKER-NONIUS, 2003)
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_computing_molecular_graphics   Olex2
_computing_publication_material 'Bruker SHELXTL'

_refine_special_details

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' Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F^2^, conventional R-factors R are based
on F, with F set to zero for negative F^2^. The threshold expression of
F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F^2^ are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
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_atom_sites_solution_secondary   difmap
_atom_sites_solution_hydrogens   geom
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'Flack H D (1983), Acta Cryst. A39, 876-881'
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Co1 Co 0.59199(3) 0.21232(2) 0.499770(16) 0.02637(9) Uani 1 1 d . B .	
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Cl2 Cl 0.69086(6) 0.41123(5) 0.37879(3) 0.03402(15) Uani 1 1 d . . .	
Cl3 Cl 0.81659(6) 0.27663(6) 0.59136(4) 0.0468(2) Uani 1 1 d . . .	
C1 C 0.4857(2) 0.0712(2) 0.55904(13) 0.0337(6) Uani 1 1 d . . .	
H1 H 0.4358 0.1212 0.5677 0.040 Uiso 1 1 calc R ..	
C2 C 0.4387(3) -0.0264(2) 0.56632(13) 0.0390(7) Uani 1 1 d . . .	
C3 C 0.4894(4) -0.1116(3) 0.55912(18) 0.0557(10) Uani 1 1 d . . .	
H3 H 0.5566 -0.1105 0.5511 0.067 Uiso 1 1 calc R ..	
C4 C 0.4402(5) -0.1991(3) 0.5638(2) 0.0690(14) Uani 1 1 d . . .	
H4 H 0.4742 -0.2580 0.5584 0.083 Uiso 1 1 calc R ..	
C5 C 0.3440(4) -0.2013(3) 0.57603(16) 0.0641(13) Uani 1 1 d . . .	
H5 H 0.3113 -0.2615 0.5787 0.077 Uiso 1 1 calc R ..	
C6 C 0.2957(4) -0.1187(3) 0.58433(17) 0.0595(11) Uani 1 1 d . . .	
H6 H 0.2291 -0.1209 0.5938 0.071 Uiso 1 1 calc R ..	
C7 C 0.3417(3) -0.0300(3) 0.57926(15) 0.0464(8) Uani 1 1 d . . .	
H7 H 0.3064 0.0281 0.5847 0.056 Uiso 1 1 calc R ..	
C8 C 0.5744(3) 0.0931(2) 0.59469(13) 0.0361(7) Uani 1 1 d . . .	
H8 H 0.6292 0.0534 0.5802 0.043 Uiso 1 1 calc R ..	
C9 C 0.5678(3) 0.0753(2) 0.65612(15) 0.0444(8) Uani 1 1 d . . .	

C10 C 0.6489(4) 0.0363(3) 0.68202(19) 0.0609(11) Uani 1 1 d . . .  
H10 H 0.7045 0.0211 0.6608 0.073 Uiso 1 1 calc R . . .  
C11 C 0.6491(4) 0.0197(4) 0.7378(2) 0.0769(15) Uani 1 1 d . . .  
H11 H 0.7043 -0.0076 0.7552 0.092 Uiso 1 1 calc R . . .  
C12 C 0.5686(5) 0.0428(4) 0.7685(2) 0.0828(19) Uani 1 1 d . . .  
H12 H 0.5690 0.0327 0.8073 0.099 Uiso 1 1 calc R . . .  
C13 C 0.4874(4) 0.0805(3) 0.74366(18) 0.0639(12) Uani 1 1 d . . .  
H13 H 0.4317 0.0953 0.7650 0.077 Uiso 1 1 calc R . . .  
C14 C 0.4877(4) 0.0968(3) 0.68688(16) 0.0524(10) Uani 1 1 d . . .  
H14 H 0.4320 0.1230 0.6694 0.063 Uiso 1 1 calc R . . .  
N1 N 0.52009(19) 0.08952(16) 0.50162(12) 0.0312(5) Uani 1 1 d . . .  
H1A H 0.5587 0.0419 0.4892 0.037 Uiso 1 1 d R . . .  
H1B H 0.4719 0.0948 0.4768 0.037 Uiso 1 1 d R . . .  
N2 N 0.59554(18) 0.19749(18) 0.58085(11) 0.0294(5) Uani 1 1 d . . .  
H2A H 0.5513 0.2412 0.5918 0.035 Uiso 1 1 d R . . .  
H2B H 0.6587 0.2092 0.5868 0.035 Uiso 1 1 d R . . .  
C1A C 0.4929(2) 0.39011(19) 0.48263(12) 0.0276(5) Uani 1 1 d . B .  
H1AA H 0.5184 0.3910 0.4440 0.033 Uiso 1 1 calc R . . .  
C2A C 0.4078(2) 0.4576(2) 0.48481(14) 0.0346(6) Uani 1 1 d . . .  
C3A C 0.3705(3) 0.4912(2) 0.53408(16) 0.0420(8) Uani 1 1 d . . .  
H3A H 0.3991 0.4718 0.5680 0.050 Uiso 1 1 calc R . . .  
C4A C 0.2917(3) 0.5532(2) 0.5345(2) 0.0527(10) Uani 1 1 d . . .  
H4A H 0.2652 0.5740 0.5686 0.063 Uiso 1 1 calc R . . .  
C5A C 0.2518(3) 0.5845(3) 0.4858(2) 0.0676(13) Uani 1 1 d . . .  
H5A H 0.1989 0.6282 0.4863 0.081 Uiso 1 1 calc R . . .  
C6A C 0.2886(4) 0.5524(4) 0.4362(3) 0.0806(17) Uani 1 1 d . . .  
H6A H 0.2621 0.5750 0.4024 0.097 Uiso 1 1 calc R . . .  
C7A C 0.3645(3) 0.4868(3) 0.4358(2) 0.0584(11) Uani 1 1 d . . .  
H7A H 0.3871 0.4616 0.4017 0.070 Uiso 1 1 calc R . . .  
C8A C 0.5775(2) 0.4131(2) 0.52143(15) 0.0357(4) Uani 1 1 d D . .  
H8A H 0.5571 0.4014 0.5605 0.043 Uiso 1 1 calc R A 1  
C9A C 0.6168(10) 0.5134(8) 0.5164(4) 0.0357(4) Uani 0.532(8) 1 d PD B 1  
C10A C 0.6748(5) 0.5460(5) 0.5590(3) 0.0357(4) Uani 0.532(8) 1 d P B 1  
H10A H 0.6820 0.5070 0.5910 0.043 Uiso 0.532(8) 1 calc PR B 1  
C11A C 0.7231(5) 0.6344(5) 0.5564(4) 0.0357(4) Uani 0.532(8) 1 d P B 1  
H11A H 0.7604 0.6568 0.5867 0.043 Uiso 0.532(8) 1 calc PR B 1  
C12A C 0.7154(5) 0.6892(4) 0.5083(4) 0.0357(4) Uani 0.532(8) 1 d P B 1  
H12A H 0.7511 0.7475 0.5046 0.043 Uiso 0.532(8) 1 calc PR B 1  
C13A C 0.6548(5) 0.6578(4) 0.4653(4) 0.0357(4) Uani 0.532(8) 1 d P B 1  
H13A H 0.6471 0.6971 0.4334 0.043 Uiso 0.532(8) 1 calc PR B 1  
C14A C 0.6061(5) 0.5703(5) 0.4687(4) 0.0357(4) Uani 0.532(8) 1 d P B 1  
H14A H 0.5660 0.5492 0.4392 0.043 Uiso 0.532(8) 1 calc PR B 1  
C9E C 0.6188(11) 0.5133(9) 0.5249(5) 0.0357(4) Uani 0.468(8) 1 d PD B 2  
C10E C 0.6558(6) 0.5441(5) 0.5770(4) 0.0357(4) Uani 0.468(8) 1 d P B 2  
H10E H 0.6476 0.5051 0.6090 0.043 Uiso 0.468(8) 1 calc PR B 2  
C11E C 0.7035(9) 0.6312(7) 0.5802(5) 0.059(3) Uani 0.468(8) 1 d P B 2

H11E H 0.7326 0.6509 0.6139 0.071 Uiso 0.468(8) 1 calc PR B 2  
C12E C 0.7087(5) 0.6897(5) 0.5343(4) 0.0357(4) Uani 0.468(8) 1 d P B 2  
H12E H 0.7415 0.7498 0.5371 0.043 Uiso 0.468(8) 1 calc PR B 2  
C13E C 0.6696(6) 0.6653(5) 0.4862(4) 0.0357(4) Uani 0.468(8) 1 d P B 2  
H13E H 0.6722 0.7089 0.4560 0.043 Uiso 0.468(8) 1 calc PR B 2  
C14E C 0.6240(6) 0.5741(6) 0.4800(4) 0.0357(4) Uani 0.468(8) 1 d P B 2  
H14E H 0.5974 0.5554 0.4454 0.043 Uiso 0.468(8) 1 calc PR B 2  
N1A N 0.46939(17) 0.28662(15) 0.49686(11) 0.0274(4) Uani 1 1 d . . .  
H1AB H 0.4376 0.2778 0.5289 0.033 Uiso 1 1 d R B .  
H1AC H 0.4326 0.2645 0.4690 0.033 Uiso 1 1 d R . .  
N2A N 0.65278(16) 0.34006(15) 0.50553(11) 0.0265(5) Uani 1 1 d . B .  
H2AA H 0.6722 0.3517 0.4707 0.032 Uiso 1 1 d R . .  
H2AB H 0.7006 0.3450 0.5305 0.032 Uiso 1 1 d R . .  
C1B C 0.7609(2) 0.1645(2) 0.43894(13) 0.0335(6) Uani 1 1 d D . .  
H1BA H 0.7792 0.2341 0.4349 0.040 Uiso 1 1 calc R C 1  
C2B C 0.8501(2) 0.1054(3) 0.43017(18) 0.0492(8) Uani 0.608(4) 1 d PD D 1  
C3B C 0.8444(8) 0.0165(13) 0.4016(8) 0.0492(8) Uani 0.608(4) 1 d P D 1  
H3B H 0.7845 -0.0137 0.3933 0.059 Uiso 0.608(4) 1 calc PR D 1  
C4B C 0.9368(6) -0.0255(6) 0.3858(3) 0.0460(15) Uani 0.608(4) 1 d P D 1  
H4B H 0.9376 -0.0800 0.3620 0.055 Uiso 0.608(4) 1 calc PR D 1  
C5B C 1.0232(5) 0.0119(6) 0.4047(3) 0.0559(15) Uani 0.608(4) 1 d P D 1  
H5B H 1.0818 -0.0217 0.3978 0.067 Uiso 0.608(4) 1 calc PR D 1  
C6B C 1.0246(4) 0.0969(5) 0.4331(3) 0.0520(13) Uani 0.608(4) 1 d P D 1  
H6B H 1.0846 0.1223 0.4454 0.062 Uiso 0.608(4) 1 calc PR D 1  
C7B C 0.9402(4) 0.1469(4) 0.4444(3) 0.0377(11) Uani 0.608(4) 1 d P D 1  
H7B H 0.9428 0.2085 0.4615 0.045 Uiso 0.608(4) 1 calc PR D 1  
C2C C 0.8501(2) 0.1054(3) 0.43017(18) 0.0492(8) Uani 0.392(4) 1 d PD D 2  
C3C C 0.8563(13) 0.020(2) 0.4022(13) 0.0492(8) Uani 0.392(4) 1 d P D 2  
H3C H 0.8076 0.0072 0.3755 0.059 Uiso 0.392(4) 1 calc PR D 2  
C4C C 0.9275(10) -0.0494(9) 0.4091(5) 0.0460(15) Uani 0.392(4) 1 d P D 2  
H4C H 0.9206 -0.1112 0.3925 0.055 Uiso 0.392(4) 1 calc PR D 2  
C5C C 1.0071(8) -0.0287(9) 0.4398(5) 0.0559(15) Uani 0.392(4) 1 d P D 2  
H5C H 1.0597 -0.0726 0.4420 0.067 Uiso 0.392(4) 1 calc PR D 2  
C6C C 1.0090(7) 0.0588(8) 0.4681(5) 0.0520(13) Uani 0.392(4) 1 d P D 2  
H6C H 1.0664 0.0773 0.4867 0.062 Uiso 0.392(4) 1 calc PR D 2  
C7C C 0.9305(7) 0.1191(7) 0.4698(4) 0.0377(11) Uani 0.392(4) 1 d P D 2  
H7C H 0.9277 0.1695 0.4963 0.045 Uiso 0.392(4) 1 calc PR D 2  
C8B C 0.6773(2) 0.1446(2) 0.39924(14) 0.0340(6) Uani 1 1 d . B .  
H8B H 0.6563 0.0761 0.4046 0.041 Uiso 1 1 calc R . .  
C9B C 0.6981(2) 0.1592(2) 0.33926(14) 0.0360(7) Uani 1 1 d . . .  
C10B C 0.6329(3) 0.1226(3) 0.30057(16) 0.0470(8) Uani 1 1 d . D .  
H10B H 0.5789 0.0858 0.3125 0.056 Uiso 1 1 calc R . .  
C11B C 0.6469(3) 0.1400(3) 0.24459(18) 0.0554(9) Uani 1 1 d . . .  
H11B H 0.6024 0.1151 0.2183 0.066 Uiso 1 1 calc R D .  
C12B C 0.7261(3) 0.1939(3) 0.22703(16) 0.0517(9) Uani 1 1 d . D .  
H12B H 0.7345 0.2075 0.1889 0.062 Uiso 1 1 calc R . .

C13B C 0.7918(3) 0.2276(3) 0.26482(15) 0.0473(8) Uani 1 1 d . . .  
 H13B H 0.8469 0.2626 0.2527 0.057 Uiso 1 1 calc R D .  
 C14B C 0.7779(3) 0.2105(2) 0.32067(15) 0.0420(7) Uani 1 1 d . D .  
 H14B H 0.8236 0.2342 0.3466 0.050 Uiso 1 1 calc R . .  
 N1B N 0.71867(18) 0.15121(16) 0.49574(12) 0.0331(5) Uani 1 1 d . B .  
 H1BB H 0.7204 0.0865 0.4994 0.040 Uiso 1 1 d R . .  
 H1BC H 0.7596 0.1694 0.5227 0.040 Uiso 1 1 d R . .  
 N2B N 0.59740(18) 0.20908(17) 0.41879(11) 0.0291(5) Uani 1 1 d . . .  
 H2BA H 0.6051 0.2684 0.4042 0.035 Uiso 1 1 d R B .  
 H2BB H 0.5417 0.1923 0.4022 0.035 Uiso 1 1 d R . .  
 C31 C 0.5138(4) 0.8703(4) 0.4192(2) 0.0716(13) Uani 1 1 d D . .  
 H31A H 0.5124 0.8475 0.3809 0.107 Uiso 1 1 calc R . .  
 H31B H 0.4628 0.9185 0.4247 0.107 Uiso 1 1 calc R . .  
 H31C H 0.5033 0.8157 0.4442 0.107 Uiso 1 1 calc R . .  
 O30 O 0.6027(2) 0.91163(19) 0.43014(12) 0.0557(7) Uani 1 1 d D . .  
 H30 H 0.6392 0.9042 0.4027 0.084 Uiso 1 1 d RD . .  
 C36 C 0.2568(4) -0.1069(4) 0.4380(2) 0.0755(14) Uani 1 1 d . . .  
 H36A H 0.2170 -0.1655 0.4369 0.113 Uiso 1 1 calc R . .  
 H36B H 0.2274 -0.0599 0.4631 0.113 Uiso 1 1 calc R . .  
 H36C H 0.3218 -0.1232 0.4510 0.113 Uiso 1 1 calc R . .  
 O35 O 0.2626(2) -0.0670(2) 0.38462(13) 0.0605(7) Uani 1 1 d . . .  
 H35 H 0.2967 -0.0168 0.3855 0.091 Uiso 1 1 calc R . .  
 O40 O 0.8834(3) 0.8738(3) 0.55684(18) 0.0857(11) Uani 1 1 d . . .  
 H40A H 0.9347 0.8945 0.5415 0.128 Uiso 1 1 d R . .  
 H40B H 0.8986 0.8319 0.5810 0.128 Uiso 1 1 d R . .  
 O50 O 0.7172(2) 0.94890(18) 0.52167(13) 0.0605(8) Uani 1 1 d . . .  
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 H50B H 0.7725 0.9277 0.5310 0.091 Uiso 1 1 d R . .

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 Cl2 0.0412(4) 0.0283(3) 0.0325(3) -0.0002(3) -0.0013(3) -0.0048(3)  
 Cl3 0.0356(4) 0.0483(5) 0.0564(5) -0.0053(4) -0.0138(3) 0.0068(3)  
 C1 0.0494(18) 0.0205(13) 0.0312(15) 0.0002(11) -0.0011(13) -0.0054(12)  
 C2 0.066(2) 0.0250(14) 0.0260(14) 0.0030(11) -0.0009(14) -0.0116(14)  
 C3 0.081(3) 0.0295(17) 0.057(2) 0.0057(15) 0.009(2) -0.0060(17)  
 C4 0.124(4) 0.0234(17) 0.060(3) 0.0017(16) 0.012(3) -0.011(2)  
 C5 0.114(4) 0.040(2) 0.039(2) 0.0039(15) 0.005(2) -0.037(2)

C6 0.085(3) 0.049(2) 0.045(2) 0.0044(17) 0.000(2) -0.029(2)  
 C7 0.064(2) 0.0401(18) 0.0346(17) 0.0039(14) 0.0024(16) -0.0164(16)  
 C8 0.0533(18) 0.0210(13) 0.0339(16) 0.0028(11) -0.0057(14) -0.0029(12)  
 C9 0.071(2) 0.0259(14) 0.0357(17) 0.0048(12) -0.0141(16) -0.0113(15)  
 C10 0.068(3) 0.060(2) 0.054(2) 0.0162(19) -0.018(2) -0.019(2)  
 C11 0.083(3) 0.086(3) 0.061(3) 0.025(3) -0.032(3) -0.023(3)  
 C12 0.134(5) 0.077(3) 0.037(2) 0.013(2) -0.030(3) -0.047(3)  
 C13 0.111(4) 0.0410(19) 0.040(2) 0.0022(16) -0.001(2) -0.018(2)  
 C14 0.091(3) 0.0317(17) 0.0350(18) 0.0040(13) -0.0023(19) -0.0075(18)  
 N1 0.0401(13) 0.0199(10) 0.0335(12) 0.0005(10) -0.0016(11) -0.0013(9)  
 N2 0.0340(13) 0.0219(11) 0.0323(13) 0.0003(9) -0.0024(10) 0.0009(9)  
 C1A 0.0291(13) 0.0203(12) 0.0332(14) 0.0015(10) 0.0014(11) -0.0017(10)  
 C2A 0.0261(13) 0.0281(13) 0.0495(19) -0.0012(12) -0.0010(12) -0.0019(11)  
 C3A 0.0427(18) 0.0260(14) 0.057(2) -0.0003(13) 0.0118(15) 0.0000(13)  
 C4A 0.049(2) 0.0272(16) 0.082(3) -0.0066(17) 0.027(2) -0.0008(14)  
 C5A 0.044(2) 0.050(2) 0.109(4) -0.007(2) -0.005(2) 0.0202(17)  
 C6A 0.073(3) 0.078(3) 0.090(4) -0.016(3) -0.035(3) 0.041(3)  
 C7A 0.053(2) 0.061(2) 0.061(3) -0.008(2) -0.0186(19) 0.0207(19)  
 C8A 0.0343(8) 0.0236(6) 0.0493(14) -0.0044(8) -0.0020(8) -0.0025(5)  
 C9A 0.0343(8) 0.0236(6) 0.0493(14) -0.0044(8) -0.0020(8) -0.0025(5)  
 C10A 0.0343(8) 0.0236(6) 0.0493(14) -0.0044(8) -0.0020(8) -0.0025(5)  
 C11A 0.0343(8) 0.0236(6) 0.0493(14) -0.0044(8) -0.0020(8) -0.0025(5)  
 C12A 0.0343(8) 0.0236(6) 0.0493(14) -0.0044(8) -0.0020(8) -0.0025(5)  
 C13A 0.0343(8) 0.0236(6) 0.0493(14) -0.0044(8) -0.0020(8) -0.0025(5)  
 C14A 0.0343(8) 0.0236(6) 0.0493(14) -0.0044(8) -0.0020(8) -0.0025(5)  
 C9E 0.0343(8) 0.0236(6) 0.0493(14) -0.0044(8) -0.0020(8) -0.0025(5)  
 C10E 0.0343(8) 0.0236(6) 0.0493(14) -0.0044(8) -0.0020(8) -0.0025(5)  
 C11E 0.078(7) 0.035(4) 0.065(7) 0.003(4) -0.016(5) -0.013(4)  
 C12E 0.0343(8) 0.0236(6) 0.0493(14) -0.0044(8) -0.0020(8) -0.0025(5)  
 C13E 0.0343(8) 0.0236(6) 0.0493(14) -0.0044(8) -0.0020(8) -0.0025(5)  
 C14E 0.0343(8) 0.0236(6) 0.0493(14) -0.0044(8) -0.0020(8) -0.0025(5)  
 N1A 0.0303(11) 0.0221(10) 0.0299(12) -0.0017(9) 0.0002(10) -0.0039(8)  
 N2A 0.0275(11) 0.0196(10) 0.0322(13) 0.0001(9) 0.0002(9) -0.0002(8)  
 C1B 0.0345(15) 0.0255(13) 0.0406(17) -0.0098(12) -0.0013(12) 0.0004(11)  
 C2B 0.0355(16) 0.0432(15) 0.0688(18) -0.0276(13) -0.0068(15) 0.0060(13)  
 C3B 0.0355(16) 0.0432(15) 0.0688(18) -0.0276(13) -0.0068(15) 0.0060(13)  
 C4B 0.052(3) 0.045(4) 0.041(4) -0.012(3) -0.007(4) 0.013(3)  
 C5B 0.043(3) 0.073(4) 0.052(3) -0.020(3) -0.005(3) 0.022(3)  
 C6B 0.033(2) 0.055(3) 0.069(4) -0.009(3) -0.010(3) -0.002(2)  
 C7B 0.041(2) 0.030(3) 0.042(3) -0.002(2) -0.009(3) 0.003(2)  
 C2C 0.0355(16) 0.0432(15) 0.0688(18) -0.0276(13) -0.0068(15) 0.0060(13)  
 C3C 0.0355(16) 0.0432(15) 0.0688(18) -0.0276(13) -0.0068(15) 0.0060(13)  
 C4C 0.052(3) 0.045(4) 0.041(4) -0.012(3) -0.007(4) 0.013(3)  
 C5C 0.043(3) 0.073(4) 0.052(3) -0.020(3) -0.005(3) 0.022(3)  
 C6C 0.033(2) 0.055(3) 0.069(4) -0.009(3) -0.010(3) -0.002(2)  
 C7C 0.041(2) 0.030(3) 0.042(3) -0.002(2) -0.009(3) 0.003(2)

C8B 0.0363(15) 0.0209(13) 0.0448(17) -0.0093(11) -0.0003(13) 0.0001(11)  
C9B 0.0411(16) 0.0259(14) 0.0412(17) -0.0115(12) 0.0004(13) 0.0019(12)  
C10B 0.053(2) 0.0392(18) 0.049(2) -0.0124(15) -0.0096(16) -0.0011(15)  
C11B 0.065(2) 0.054(2) 0.047(2) -0.0178(18) -0.0123(19) 0.0011(18)  
C12B 0.074(3) 0.0419(18) 0.0390(18) -0.0081(15) -0.0015(17) 0.0077(18)  
C13B 0.062(2) 0.0387(18) 0.041(2) -0.0119(14) 0.0069(15) 0.0073(16)  
C14B 0.0491(19) 0.0383(17) 0.0387(18) -0.0134(13) 0.0037(14) -0.0018(14)  
N1B 0.0399(13) 0.0223(10) 0.0373(14) -0.0032(10) -0.0061(11) 0.0044(9)  
N2B 0.0301(12) 0.0233(11) 0.0339(14) -0.0022(9) 0.0003(10) 0.0005(9)  
C31 0.069(3) 0.084(3) 0.061(3) -0.023(2) -0.006(2) 0.005(3)  
O30 0.0691(18) 0.0461(14) 0.0519(16) -0.0107(12) 0.0109(13) -0.0055(13)  
C36 0.076(3) 0.088(4) 0.063(3) 0.020(3) 0.006(2) 0.008(3)  
O35 0.0651(18) 0.0583(17) 0.0580(17) -0.0067(13) -0.0046(14) -0.0137(14)  
O40 0.088(3) 0.069(2) 0.100(3) 0.018(2) -0.007(2) -0.0098(19)  
O50 0.089(2) 0.0310(12) 0.0610(17) 0.0024(11) -0.0037(15) 0.0136(13)

\_geom\_special\_details

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All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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loop\_

\_geom\_bond\_atom\_site\_label\_1  
\_geom\_bond\_atom\_site\_label\_2  
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\_geom\_bond\_site\_symmetry\_2  
\_geom\_bond\_publ\_flag

Co1 N1B 1.949(3) . ?

Co1 N2A 1.963(2) . ?

Co1 N2B 1.963(3) . ?

Co1 N1 1.970(2) . ?

Co1 N2 1.975(3) . ?

Co1 N1A 1.985(2) . ?

C1 N1 1.492(4) . ?

C1 C2 1.509(4) . ?

C1 C8 1.531(5) . ?

C1 H1 1.0000 . ?

C2 C7 1.380(6) . ?

C2 C3 1.384(5) . ?

C3 C4 1.393(6) . ?

C3 H3 0.9500 . ?

C4 C5 1.364(8) . ?  
C4 H4 0.9500 . ?  
C5 C6 1.340(7) . ?  
C5 H5 0.9500 . ?  
C6 C7 1.388(5) . ?  
C6 H6 0.9500 . ?  
C7 H7 0.9500 . ?  
C8 C9 1.511(5) . ?  
C8 N2 1.511(4) . ?  
C8 H8 1.0000 . ?  
C9 C14 1.369(6) . ?  
C9 C10 1.394(6) . ?  
C10 C11 1.371(7) . ?  
C10 H10 0.9500 . ?  
C11 C12 1.377(9) . ?  
C11 H11 0.9500 . ?  
C12 C13 1.378(8) . ?  
C12 H12 0.9500 . ?  
C13 C14 1.393(6) . ?  
C13 H13 0.9500 . ?  
C14 H14 0.9500 . ?  
N1 H1A 0.8999 . ?  
N1 H1B 0.9000 . ?  
N2 H2A 0.8998 . ?  
N2 H2B 0.9000 . ?  
C1A C2A 1.504(4) . ?  
C1A N1A 1.509(3) . ?  
C1A C8A 1.535(4) . ?  
C1A H1AA 1.0000 . ?  
C2A C3A 1.381(5) . ?  
C2A C7A 1.389(5) . ?  
C3A C4A 1.388(5) . ?  
C3A H3A 0.9500 . ?  
C4A C5A 1.372(7) . ?  
C4A H4A 0.9500 . ?  
C5A C6A 1.378(8) . ?  
C5A H5A 0.9500 . ?  
C6A C7A 1.388(6) . ?  
C6A H6A 0.9500 . ?  
C7A H7A 0.9500 . ?  
C8A C9A 1.495(10) . ?  
C8A N2A 1.502(4) . ?  
C8A C9E 1.502(11) . ?  
C8A H8A 1.0000 . ?  
C9A C10A 1.381(11) . ?  
C9A C14A 1.406(12) . ?

C10A C11A 1.396(9) . ?  
C10A H10A 0.9500 . ?  
C11A C12A 1.393(11) . ?  
C11A H11A 0.9500 . ?  
C12A C13A 1.405(9) . ?  
C12A H12A 0.9500 . ?  
C13A C14A 1.389(9) . ?  
C13A H13A 0.9500 . ?  
C14A H14A 0.9500 . ?  
C9E C14E 1.377(14) . ?  
C9E C10E 1.426(13) . ?  
C10E C11E 1.376(11) . ?  
C10E H10E 0.9500 . ?  
C11E C12E 1.377(13) . ?  
C11E H11E 0.9500 . ?  
C12E C13E 1.327(11) . ?  
C12E H12E 0.9500 . ?  
C13E C14E 1.419(10) . ?  
C13E H13E 0.9500 . ?  
C14E H14E 0.9500 . ?  
N1A H1AB 0.9000 . ?  
N1A H1AC 0.8999 . ?  
N2A H2AA 0.9003 . ?  
N2A H2AB 0.8999 . ?  
C1B C2B 1.495(3) . ?  
C1B N1B 1.506(4) . ?  
C1B C8B 1.530(4) . ?  
C1B H1BA 1.0000 . ?  
C2B C3B 1.414(16) . ?  
C2B C7B 1.416(7) . ?  
C3B C4B 1.456(16) . ?  
C3B H3B 0.9500 . ?  
C4B C5B 1.381(11) . ?  
C4B H4B 0.9500 . ?  
C5B C6B 1.364(10) . ?  
C5B H5B 0.9500 . ?  
C6B C7B 1.384(9) . ?  
C6B H6B 0.9500 . ?  
C7B H7B 0.9500 . ?  
C3C C4C 1.39(3) . ?  
C3C H3C 0.9500 . ?  
C4C C5C 1.360(17) . ?  
C4C H4C 0.9500 . ?  
C5C C6C 1.390(15) . ?  
C5C H5C 0.9500 . ?  
C6C C7C 1.370(14) . ?

C6C H6C 0.9500 . ?  
C7C H7C 0.9500 . ?  
C8B C9B 1.494(5) . ?  
C8B N2B 1.498(4) . ?  
C8B H8B 1.0000 . ?  
C9B C14B 1.388(5) . ?  
C9B C10B 1.396(5) . ?  
C10B C11B 1.390(6) . ?  
C10B H10B 0.9500 . ?  
C11B C12B 1.392(6) . ?  
C11B H11B 0.9500 . ?  
C12B C13B 1.372(6) . ?  
C12B H12B 0.9500 . ?  
C13B C14B 1.386(5) . ?  
C13B H13B 0.9500 . ?  
C14B H14B 0.9500 . ?  
N1B H1BB 0.9001 . ?  
N1B H1BC 0.9002 . ?  
N2B H2BA 0.8998 . ?  
N2B H2BB 0.9002 . ?  
C31 O30 1.381(6) . ?  
C31 H31A 0.9800 . ?  
C31 H31B 0.9800 . ?  
C31 H31C 0.9800 . ?  
O30 H30 0.8401 . ?  
C36 O35 1.408(6) . ?  
C36 H36A 0.9800 . ?  
C36 H36B 0.9800 . ?  
C36 H36C 0.9800 . ?  
O35 H35 0.8400 . ?  
O40 H40A 0.8500 . ?  
O40 H40B 0.8499 . ?  
O50 H50A 0.8496 . ?  
O50 H50B 0.8502 . ?

loop\_  
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  \_geom\_angle\_atom\_site\_label\_3  
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N1B Co1 N2A 90.50(10) . . ?  
N1B Co1 N2B 84.59(11) . . ?  
N2A Co1 N2B 94.32(10) . . ?

N1B Co1 N1 94.66(10) . . ?  
N2A Co1 N1 172.73(11) . . ?  
N2B Co1 N1 91.28(11) . . ?  
N1B Co1 N2 88.99(11) . . ?  
N2A Co1 N2 90.70(10) . . ?  
N2B Co1 N2 171.88(9) . . ?  
N1 Co1 N2 84.28(11) . . ?  
N1B Co1 N1A 172.65(11) . . ?  
N2A Co1 N1A 84.40(9) . . ?  
N2B Co1 N1A 90.51(10) . . ?  
N1 Co1 N1A 90.91(10) . . ?  
N2 Co1 N1A 96.34(11) . . ?  
N1 C1 C2 113.5(2) . . ?  
N1 C1 C8 103.6(3) . . ?  
C2 C1 C8 117.2(3) . . ?  
N1 C1 H1 107.3 . . ?  
C2 C1 H1 107.3 . . ?  
C8 C1 H1 107.3 . . ?  
C7 C2 C3 119.4(3) . . ?  
C7 C2 C1 118.6(3) . . ?  
C3 C2 C1 122.0(4) . . ?  
C2 C3 C4 118.9(5) . . ?  
C2 C3 H3 120.6 . . ?  
C4 C3 H3 120.6 . . ?  
C5 C4 C3 120.9(4) . . ?  
C5 C4 H4 119.5 . . ?  
C3 C4 H4 119.5 . . ?  
C6 C5 C4 120.1(4) . . ?  
C6 C5 H5 120.0 . . ?  
C4 C5 H5 120.0 . . ?  
C5 C6 C7 120.8(5) . . ?  
C5 C6 H6 119.6 . . ?  
C7 C6 H6 119.6 . . ?  
C2 C7 C6 119.9(4) . . ?  
C2 C7 H7 120.1 . . ?  
C6 C7 H7 120.1 . . ?  
C9 C8 N2 112.7(2) . . ?  
C9 C8 C1 118.3(3) . . ?  
N2 C8 C1 102.7(2) . . ?  
C9 C8 H8 107.5 . . ?  
N2 C8 H8 107.5 . . ?  
C1 C8 H8 107.5 . . ?  
C14 C9 C10 119.4(4) . . ?  
C14 C9 C8 123.3(3) . . ?  
C10 C9 C8 117.2(4) . . ?  
C11 C10 C9 120.7(5) . . ?

C11 C10 H10 119.7 . . ?  
C9 C10 H10 119.7 . . ?  
C10 C11 C12 119.4(5) . . ?  
C10 C11 H11 120.3 . . ?  
C12 C11 H11 120.3 . . ?  
C11 C12 C13 120.8(4) . . ?  
C11 C12 H12 119.6 . . ?  
C13 C12 H12 119.6 . . ?  
C12 C13 C14 119.4(5) . . ?  
C12 C13 H13 120.3 . . ?  
C14 C13 H13 120.3 . . ?  
C9 C14 C13 120.3(4) . . ?  
C9 C14 H14 119.9 . . ?  
C13 C14 H14 119.9 . . ?  
C1 N1 Co1 109.22(18) . . ?  
C1 N1 H1A 112.2 . . ?  
Co1 N1 H1A 108.9 . . ?  
C1 N1 H1B 113.6 . . ?  
Co1 N1 H1B 106.8 . . ?  
H1A N1 H1B 106.0 . . ?  
C8 N2 Co1 108.36(19) . . ?  
C8 N2 H2A 116.4 . . ?  
Co1 N2 H2A 101.9 . . ?  
C8 N2 H2B 108.9 . . ?  
Co1 N2 H2B 99.4 . . ?  
H2A N2 H2B 119.5 . . ?  
C2A C1A N1A 114.3(2) . . ?  
C2A C1A C8A 116.6(2) . . ?  
N1A C1A C8A 102.8(2) . . ?  
C2A C1A H1AA 107.5 . . ?  
N1A C1A H1AA 107.5 . . ?  
C8A C1A H1AA 107.5 . . ?  
C3A C2A C7A 118.6(3) . . ?  
C3A C2A C1A 122.1(3) . . ?  
C7A C2A C1A 119.2(3) . . ?  
C2A C3A C4A 120.5(4) . . ?  
C2A C3A H3A 119.7 . . ?  
C4A C3A H3A 119.7 . . ?  
C5A C4A C3A 120.4(4) . . ?  
C5A C4A H4A 119.8 . . ?  
C3A C4A H4A 119.8 . . ?  
C4A C5A C6A 119.9(4) . . ?  
C4A C5A H5A 120.1 . . ?  
C6A C5A H5A 120.1 . . ?  
C5A C6A C7A 119.7(5) . . ?  
C5A C6A H6A 120.1 . . ?

C7A C6A H6A 120.1 . . ?  
C6A C7A C2A 120.7(4) . . ?  
C6A C7A H7A 119.6 . . ?  
C2A C7A H7A 119.6 . . ?  
C9A C8A N2A 110.6(6) . . ?  
C9A C8A C9E 7.9(8) . . ?  
N2A C8A C9E 111.9(7) . . ?  
C9A C8A C1A 114.9(5) . . ?  
N2A C8A C1A 103.4(2) . . ?  
C9E C8A C1A 121.1(6) . . ?  
C9A C8A H8A 109.2 . . ?  
N2A C8A H8A 109.2 . . ?  
C9E C8A H8A 101.8 . . ?  
C1A C8A H8A 109.2 . . ?  
C10A C9A C14A 119.4(8) . . ?  
C10A C9A C8A 117.0(8) . . ?  
C14A C9A C8A 123.2(7) . . ?  
C9A C10A C11A 122.1(7) . . ?  
C9A C10A H10A 119.0 . . ?  
C11A C10A H10A 119.0 . . ?  
C12A C11A C10A 118.6(7) . . ?  
C12A C11A H11A 120.7 . . ?  
C10A C11A H11A 120.7 . . ?  
C11A C12A C13A 119.7(6) . . ?  
C11A C12A H12A 120.1 . . ?  
C13A C12A H12A 120.1 . . ?  
C14A C13A C12A 121.0(6) . . ?  
C14A C13A H13A 119.5 . . ?  
C12A C13A H13A 119.5 . . ?  
C13A C14A C9A 119.1(6) . . ?  
C13A C14A H14A 120.5 . . ?  
C9A C14A H14A 120.5 . . ?  
C14E C9E C10E 119.9(9) . . ?  
C14E C9E C8A 122.6(8) . . ?  
C10E C9E C8A 117.5(8) . . ?  
C11E C10E C9E 118.9(8) . . ?  
C11E C10E H10E 120.6 . . ?  
C9E C10E H10E 120.6 . . ?  
C10E C11E C12E 119.7(9) . . ?  
C10E C11E H11E 120.2 . . ?  
C12E C11E H11E 120.2 . . ?  
C13E C12E C11E 122.5(7) . . ?  
C13E C12E H12E 118.8 . . ?  
C11E C12E H12E 118.8 . . ?  
C12E C13E C14E 120.1(7) . . ?  
C12E C13E H13E 120.0 . . ?

C14E C13E H13E 120.0 . . ?  
C9E C14E C13E 118.8(8) . . ?  
C9E C14E H14E 120.6 . . ?  
C13E C14E H14E 120.6 . . ?  
C1A N1A Co1 108.37(16) . . ?  
C1A N1A H1AB 115.5 . . ?  
Co1 N1A H1AB 108.4 . . ?  
C1A N1A H1AC 105.9 . . ?  
Co1 N1A H1AC 109.5 . . ?  
H1AB N1A H1AC 108.9 . . ?  
C8A N2A Co1 109.12(17) . . ?  
C8A N2A H2AA 109.0 . . ?  
Co1 N2A H2AA 102.9 . . ?  
C8A N2A H2AB 106.7 . . ?  
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H2AA N2A H2AB 113.5 . . ?  
C2B C1B N1B 112.5(3) . . ?  
C2B C1B C8B 115.9(3) . . ?  
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C2B C1B H1BA 107.7 . . ?  
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C8B C1B H1BA 107.7 . . ?  
C3B C2B C7B 121.4(6) . . ?  
C3B C2B C1B 120.0(5) . . ?  
C7B C2B C1B 118.1(3) . . ?  
C2B C3B C4B 115.3(8) . . ?  
C2B C3B H3B 122.3 . . ?  
C4B C3B H3B 122.3 . . ?  
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C3B C4B H4B 119.2 . . ?  
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C14B C9B C8B 122.5(3) . . ?  
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C11B C10B C9B 120.1(4) . . ?  
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C9B C14B H14B 119.5 . . ?  
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Co1 N1B H1BC 114.1 . . ?  
H1BB N1B H1BC 100.9 . . ?  
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C8B N2B H2BA 109.4 . . ?  
Co1 N2B H2BA 112.1 . . ?  
C8B N2B H2BB 109.7 . . ?  
Co1 N2B H2BB 114.9 . . ?  
H2BA N2B H2BB 99.2 . . ?  
O30 C31 H31A 109.5 . . ?  
O30 C31 H31B 109.5 . . ?  
H31A C31 H31B 109.5 . . ?  
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H31A C31 H31C 109.5 . . ?

H31B C31 H31C 109.5 . . ?  
C31 O30 H30 109.5 . . ?  
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H36B C36 H36C 109.5 . . ?  
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C7 C2 C3 C4 1.6(6) . . . ?  
C1 C2 C3 C4 -176.8(4) . . . ?  
C2 C3 C4 C5 -1.0(7) . . . ?  
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C3 C2 C7 C6 -0.7(5) . . . ?  
C1 C2 C7 C6 177.8(3) . . . ?  
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C2 C1 C8 N2 -174.8(3) . . . ?  
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C14 C9 C10 C11 -0.2(6) . . . ?  
C8 C9 C10 C11 178.8(4) . . . ?  
C9 C10 C11 C12 -0.7(7) . . . ?

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C11 C12 C13 C14 -1.1(7) . . . ?  
C10 C9 C14 C13 0.4(5) . . . ?  
C8 C9 C14 C13 -178.5(3) . . . ?  
C12 C13 C14 C9 0.2(6) . . . ?  
C2 C1 N1 Co1 -173.9(2) . . . ?  
C8 C1 N1 Co1 -45.7(2) . . . ?  
N1B Co1 N1 C1 104.4(2) . . . ?  
N2A Co1 N1 C1 -30.7(10) . . . ?  
N2B Co1 N1 C1 -171.0(2) . . . ?  
N2 Co1 N1 C1 15.8(2) . . . ?  
N1A Co1 N1 C1 -80.4(2) . . . ?  
C9 C8 N2 Co1 -175.6(2) . . . ?  
C1 C8 N2 Co1 -47.2(3) . . . ?  
N1B Co1 N2 C8 -76.4(2) . . . ?  
N2A Co1 N2 C8 -166.8(2) . . . ?  
N2B Co1 N2 C8 -38.7(8) . . . ?  
N1 Co1 N2 C8 18.4(2) . . . ?  
N1A Co1 N2 C8 108.7(2) . . . ?  
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C5A C6A C7A C2A -4.0(8) . . . ?  
C3A C2A C7A C6A 3.3(6) . . . ?  
C1A C2A C7A C6A -177.1(4) . . . ?  
C2A C1A C8A C9A -54.0(6) . . . ?  
N1A C1A C8A C9A -179.9(6) . . . ?  
C2A C1A C8A N2A -174.7(2) . . . ?  
N1A C1A C8A N2A 59.4(3) . . . ?  
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N2A C8A C9A C10A -79.5(10) . . . ?  
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N2A C8A C9A C14A 93.4(11) . . . ?  
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C1A C8A C9A C14A -23.2(13) . . . ?  
C14A C9A C10A C11A 0.4(15) . . . ?  
C8A C9A C10A C11A 173.6(8) . . . ?  
C9A C10A C11A C12A -2.7(12) . . . ?

C10A C11A C12A C13A 4.2(10) . . . ?  
C11A C12A C13A C14A -3.4(10) . . . ?  
C12A C13A C14A C9A 1.0(12) . . . ?  
C10A C9A C14A C13A 0.5(15) . . . ?  
C8A C9A C14A C13A -172.2(9) . . . ?  
C9A C8A C9E C14E 5(7) . . . ?  
N2A C8A C9E C14E 88.0(13) . . . ?  
C1A C8A C9E C14E -34.3(16) . . . ?  
C9A C8A C9E C10E -173(9) . . . ?  
N2A C8A C9E C10E -90.5(12) . . . ?  
C1A C8A C9E C10E 147.2(9) . . . ?  
C14E C9E C10E C11E -5.5(18) . . . ?  
C8A C9E C10E C11E 173.0(10) . . . ?  
C9E C10E C11E C12E 4.5(16) . . . ?  
C10E C11E C12E C13E -0.4(15) . . . ?  
C11E C12E C13E C14E -2.8(13) . . . ?  
C10E C9E C14E C13E 2.4(17) . . . ?  
C8A C9E C14E C13E -176.1(10) . . . ?  
C12E C13E C14E C9E 1.7(13) . . . ?  
C2A C1A N1A Co1 -173.9(2) . . . ?  
C8A C1A N1A Co1 -46.6(2) . . . ?  
N1B Co1 N1A C1A -28.7(10) . . . ?  
N2A Co1 N1A C1A 17.54(19) . . . ?  
N2B Co1 N1A C1A -76.75(19) . . . ?  
N1 Co1 N1A C1A -168.03(18) . . . ?  
N2 Co1 N1A C1A 107.62(19) . . . ?  
C9A C8A N2A Co1 -169.9(4) . . . ?  
C9E C8A N2A Co1 -178.3(5) . . . ?  
C1A C8A N2A Co1 -46.4(3) . . . ?  
N1B Co1 N2A C8A -168.5(2) . . . ?  
N2B Co1 N2A C8A 106.9(2) . . . ?  
N1 Co1 N2A C8A -33.3(10) . . . ?  
N2 Co1 N2A C8A -79.5(2) . . . ?  
N1A Co1 N2A C8A 16.8(2) . . . ?  
N1B C1B C2B C3B 99.2(10) . . . ?  
C8B C1B C2B C3B -21.6(11) . . . ?  
N1B C1B C2B C7B -89.3(5) . . . ?  
C8B C1B C2B C7B 150.0(4) . . . ?  
C7B C2B C3B C4B -3.0(19) . . . ?  
C1B C2B C3B C4B 168.3(9) . . . ?  
C2B C3B C4B C5B 9(2) . . . ?  
C3B C4B C5B C6B -8.3(15) . . . ?  
C4B C5B C6B C7B 0.8(12) . . . ?  
C5B C6B C7B C2B 5.2(11) . . . ?  
C3B C2B C7B C6B -3.9(13) . . . ?  
C1B C2B C7B C6B -175.4(5) . . . ?

C3C C4C C5C C6C 7(2) . . . ?  
C4C C5C C6C C7C 6.2(19) . . . ?  
C2B C1B C8B C9B -59.1(4) . . . ?  
N1B C1B C8B C9B 176.1(2) . . . ?  
C2B C1B C8B N2B 177.4(3) . . . ?  
N1B C1B C8B N2B 52.6(3) . . . ?  
N2B C8B C9B C14B 103.8(3) . . . ?  
C1B C8B C9B C14B -16.0(4) . . . ?  
N2B C8B C9B C10B -74.0(3) . . . ?  
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C14B C9B C10B C11B -1.8(5) . . . ?  
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C11B C12B C13B C14B -2.0(6) . . . ?  
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C10B C9B C14B C13B 1.7(5) . . . ?  
C8B C9B C14B C13B -176.1(3) . . . ?  
C2B C1B N1B Co1 -170.3(2) . . . ?  
C8B C1B N1B Co1 -43.4(2) . . . ?  
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N2B Co1 N1B C1B 17.50(18) . . . ?  
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N1A Co1 N1B C1B -30.9(9) . . . ?  
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N1 Co1 N2B C8B -81.25(19) . . . ?  
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====END

data\_jgb **Delta-(S,S)-3<sup>3+</sup> 3Cl<sup>-</sup>**

# start Validation Reply Form

\_vrf\_THETM01\_jgb

; PROBLEM: The value of sine(theta\_max)/wavelength is less than 0.575  
RESPONSE: Data was collected on a Bruker GADDS instrument with Cu-source and MWPC (multiwire proportional counter) detector. Under these experimental conditions the maximum angle that can be collected is 120 degrees two-theta.

\_vrf\_PLAT213\_jgb

; PROBLEM: Atom C1 has ADP max/min Ratio ..... 9.8  
RESPONSE: Given the complexity of the molecule with large number of water of hydration, and possibility of disorder of the peripheral phenyl groups, several atoms had NPDs. Many restraints were used to fix this and yet resulted in some of the atoms with elongated or disc shaped thermal motions. No efforts were taken to further add any restraints.

\_vrf\_PLAT415\_jgb

; PROBLEM: Short Inter D-H..H-X H1D .. H77 .. 1.83  
RESPONSE: Water molecules for which the hydrogen atoms could not be located were placed geometrically only to satisfy the stoichiometry. This results in short H - H interactions.  
No efforts were made to relocate the hydrogen atoms.

\_vrf\_PLAT417\_jgb

; PROBLEM: Short Inter D-H..H-D H2A .. H12C .. 1.62  
RESPONSE: Water molecules for which the hydrogen atoms could not be located were placed geometrically only to satisfy the stoichiometry. This results in short H - H interactions.  
No efforts were made to relocate the hydrogen atoms.

\_vrf\_PLAT220\_jgb

; PROBLEM: Large Non-Solvent C Ueq(max)/Ueq(min) ... 5.2  
RESPONSE: Given the complexity of the molecule with large number of water of hydration, and possibility of disorder of the peripheral phenyl groups, several atoms had NPDs. Many restraints were used to fix this and yet resulted in some of the atoms with elongated or disc shaped thermal motions. No efforts were taken to further add any restraints.

\_vrf\_PLAT420\_jgb  
;  
PROBLEM: D-H Without Acceptor O1 - H1C ... ?  
RESPONSE: Water molecules for which the hydrogen atoms could not be located were placed geometrically only to satisfy the stoichiometry. This results in short H - H interactions.  
No efforts were made to relocate the hydrogen atoms.  
;  
\_vrf\_PLAT860\_jgb  
;  
PROBLEM: Number of Least-Squares Restraints ..... 265  
RESPONSE: Following restraints were used  
DELU C22 C15 N3 C2 C6 C31 C30 C32 C33 C7 C3 C8 C9 C10 N6 N5  
DELU C51 C52 C56 C50 C66 C65 C70 C72 C77 C73 C71 C44 C49 C48 C45  
SIMU 0.005 0.02 1.7 C22 C15 N3 C2 C6 C31 C30 C32 C33 C7 C3 C8 C9 C10 N6 N5  
SIMU 0.005 0.02 1.7 C51 C52 C56 C50 C66 C65 C70 C72 C77 C73 C71 C44 C49 C48  
C45  
SIMU 0.005 0.01 1.7 C80 C79 C84 C73 C72 C77  
SIMU 0.005 0.01 1.7 C56 C51 C52  
SIMU 0.005 0.01 1.7 N5 C29 Co1 N6 N1 N4 N3 C15 C24 C25 C27 C2 C7 C3 C1 C8 C9  
=  
C10  
SIMU 0.005 0.01 1.7 N7 C43 C44 C51 C50 N8  
ISOR 0.005 0.01 N1 N6 C15 C25 C51 C72  
EADP N1 N6 C15 C25 C51 C72 N7 C58 N3 N5 N10 C22  
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'O' 'O' 0.0492 0.0322  
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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\_symmetry\_space\_group\_name\_H-M P2(1)

loop\_  
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  '-x, y+1/2, -z'

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_cell_angle_gamma	90.00
_cell_volume	5103.4(5)
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_cell_measurement_temperature	110(2)
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CELL-NOW (Sheldrick, 2003) and SAINT (BRUKER-NONIUS, 2003)
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_computing_publication_material 'Bruker SHELXTL'

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    Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
    goodness of fit S are based on F^2^, conventional R-factors R are based
    on F, with F set to zero for negative F^2^. The threshold expression of
    F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
    not relevant to the choice of reflections for refinement. R-factors based
    on F^2^ are statistically about twice as large as those based on F, and R-
    factors based on ALL data will be even larger.
;

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_refine_ls_weighting_details
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_atom_sites_solution_secondary   difmap
_atom_sites_solution_hydrogens   geom
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'Flack H D (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack   0.069(5)
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Co1 Co 0.60895(8) 0.59241(5) 0.32429(6) 0.0073(2) Uani 1 1 d . . .  
N1 N 0.6495(4) 0.5921(3) 0.4368(3) 0.0102(4) Uani 1 1 d U . .  
H1A H 0.6553 0.5574 0.4543 0.012 Uiso 1 1 calc R . .  
H1B H 0.7175 0.6081 0.4437 0.012 Uiso 1 1 calc R . .  
N2 N 0.5046(5) 0.6488(2) 0.3532(3) 0.0091(13) Uani 1 1 d . . .  
H2A H 0.5106 0.6768 0.3181 0.011 Uiso 1 1 calc R . .  
H2B H 0.4334 0.6359 0.3496 0.011 Uiso 1 1 calc R . .  
N3 N 0.7225(5) 0.6458(2) 0.3019(3) 0.0102(4) Uani 1 1 d U . .  
H3A H 0.7159 0.6735 0.3372 0.012 Uiso 1 1 calc R . .  
H3B H 0.7912 0.6307 0.3097 0.012 Uiso 1 1 calc R . .  
N4 N 0.5729(4) 0.5989(3) 0.2111(3) 0.0123(13) Uani 1 1 d . . .  
H4A H 0.5561 0.5658 0.1907 0.015 Uiso 1 1 calc R . .  
H4B H 0.5115 0.6203 0.2045 0.015 Uiso 1 1 calc R . .  
N5 N 0.7107(5) 0.5333(2) 0.3039(3) 0.0102(4) Uani 1 1 d U . .  
H5A H 0.7506 0.5407 0.2591 0.012 Uiso 1 1 calc R . .  
H5B H 0.7598 0.5302 0.3460 0.012 Uiso 1 1 calc R . .  
N6 N 0.4981(5) 0.5360(2) 0.3389(3) 0.0102(4) Uani 1 1 d U . .  
H6A H 0.4598 0.5426 0.3847 0.012 Uiso 1 1 calc R . .  
H6B H 0.4483 0.5369 0.2970 0.012 Uiso 1 1 calc R . .  
C1 C 0.5651(6) 0.6211(3) 0.4857(4) 0.0106(12) Uani 1 1 d U . .  
H1 H 0.5002 0.5968 0.4927 0.013 Uiso 1 1 calc R . .  
C2 C 0.6090(6) 0.6357(3) 0.5668(4) 0.0135(12) Uani 1 1 d U . .  
C3 C 0.5737(6) 0.6094(3) 0.6349(4) 0.0151(14) Uani 1 1 d U . .  
H3 H 0.5205 0.5817 0.6300 0.018 Uiso 1 1 calc R . .  
C4 C 0.6140(6) 0.6226(4) 0.7080(4) 0.0212(19) Uani 1 1 d . . .  
H4 H 0.5881 0.6041 0.7533 0.025 Uiso 1 1 calc R . .  
C5 C 0.6917(6) 0.6624(3) 0.7181(4) 0.0181(18) Uani 1 1 d . . .  
H5 H 0.7183 0.6715 0.7698 0.022 Uiso 1 1 calc R . .  
C6 C 0.7306(6) 0.6890(4) 0.6513(4) 0.0218(16) Uani 1 1 d U . .  
H6 H 0.7852 0.7160 0.6569 0.026 Uiso 1 1 calc R . .  
C7 C 0.6887(6) 0.6756(3) 0.5762(5) 0.0192(14) Uani 1 1 d U . .  
H7 H 0.7147 0.6938 0.5307 0.023 Uiso 1 1 calc R . .  
C8 C 0.5271(6) 0.6683(3) 0.4358(4) 0.0117(13) Uani 1 1 d U . .  
H8 H 0.5892 0.6946 0.4339 0.014 Uiso 1 1 calc R . .  
C9 C 0.4285(6) 0.6955(3) 0.4730(4) 0.0123(13) Uani 1 1 d U . .  
C10 C 0.3258(6) 0.6708(3) 0.4742(5) 0.0206(16) Uani 1 1 d U . .  
H10 H 0.3160 0.6372 0.4489 0.025 Uiso 1 1 calc R . .  
C11 C 0.2371(7) 0.6948(3) 0.5119(5) 0.026(2) Uani 1 1 d . . .  
H11 H 0.1666 0.6780 0.5114 0.031 Uiso 1 1 calc R . .  
C12 C 0.2519(8) 0.7425(4) 0.5496(5) 0.031(2) Uani 1 1 d . . .  
H12 H 0.1917 0.7588 0.5759 0.037 Uiso 1 1 calc R . .

C13 C 0.3527(7) 0.7666(3) 0.5498(5) 0.024(2) Uani 1 1 d . . .  
H13 H 0.3629 0.7993 0.5775 0.028 Uiso 1 1 calc R . .  
C14 C 0.4403(7) 0.7442(3) 0.5103(5) 0.0230(19) Uani 1 1 d . . .  
H14 H 0.5092 0.7624 0.5088 0.028 Uiso 1 1 calc R . .  
C15 C 0.7143(6) 0.6671(3) 0.2186(4) 0.0102(4) Uani 1 1 d U . .  
H15 H 0.6613 0.6977 0.2177 0.012 Uiso 1 1 calc R . .  
C16 C 0.8254(5) 0.6864(3) 0.1889(4) 0.0091(15) Uani 1 1 d . . .  
C17 C 0.8305(6) 0.7322(3) 0.1449(6) 0.027(2) Uani 1 1 d . . .  
H17 H 0.7652 0.7526 0.1360 0.033 Uiso 1 1 calc R . .  
C18 C 0.9300(7) 0.7494(4) 0.1130(6) 0.042(3) Uani 1 1 d . . .  
H18 H 0.9321 0.7804 0.0807 0.050 Uiso 1 1 calc R . .  
C19 C 1.0251(7) 0.7210(4) 0.1288(6) 0.031(2) Uani 1 1 d . . .  
H19 H 1.0943 0.7330 0.1096 0.037 Uiso 1 1 calc R . .  
C20 C 1.0186(6) 0.6752(3) 0.1724(5) 0.0206(18) Uani 1 1 d . . .  
H20 H 1.0841 0.6554 0.1830 0.025 Uiso 1 1 calc R . .  
C21 C 0.9200(6) 0.6572(4) 0.2013(5) 0.0205(18) Uani 1 1 d . . .  
H21 H 0.9173 0.6246 0.2298 0.025 Uiso 1 1 calc R . .  
C22 C 0.6661(6) 0.6219(3) 0.1672(4) 0.0102(4) Uani 1 1 d U . .  
H22 H 0.7242 0.5938 0.1624 0.012 Uiso 1 1 calc R . .  
C23 C 0.6347(5) 0.6403(3) 0.0834(4) 0.0083(15) Uani 1 1 d . . .  
C24 C 0.5471(6) 0.6747(3) 0.0709(4) 0.0130(14) Uani 1 1 d U . .  
H24 H 0.5076 0.6886 0.1146 0.016 Uiso 1 1 calc R . .  
C25 C 0.5169(6) 0.6890(3) -0.0073(4) 0.0102(4) Uani 1 1 d U . .  
H25 H 0.4567 0.7128 -0.0158 0.012 Uiso 1 1 calc R . .  
C26 C 0.5724(6) 0.6693(3) -0.0717(4) 0.0177(18) Uani 1 1 d . . .  
H26 H 0.5505 0.6788 -0.1243 0.021 Uiso 1 1 calc R . .  
C27 C 0.6615(6) 0.6351(3) -0.0582(5) 0.0199(18) Uani 1 1 d . . .  
H27 H 0.7028 0.6222 -0.1018 0.024 Uiso 1 1 calc R . .  
C28 C 0.6905(6) 0.6196(3) 0.0193(4) 0.0149(17) Uani 1 1 d . . .  
H28 H 0.7488 0.5948 0.0279 0.018 Uiso 1 1 calc R . .  
C29 C 0.6509(6) 0.4819(3) 0.2927(4) 0.0100(13) Uani 1 1 d U . .  
H29 H 0.6250 0.4805 0.2360 0.012 Uiso 1 1 calc R . .  
C30 C 0.7238(6) 0.4347(3) 0.3063(4) 0.0142(14) Uani 1 1 d U . .  
C31 C 0.7389(6) 0.3962(3) 0.2478(5) 0.0200(14) Uani 1 1 d U . .  
H31 H 0.7048 0.4005 0.1970 0.024 Uiso 1 1 calc R . .  
C32 C 0.8037(7) 0.3518(3) 0.2637(5) 0.0240(14) Uani 1 1 d U . .  
H32 H 0.8106 0.3250 0.2242 0.029 Uiso 1 1 calc R . .  
C33 C 0.8585(7) 0.3457(3) 0.3360(5) 0.0254(17) Uani 1 1 d U . .  
H33 H 0.9050 0.3158 0.3453 0.031 Uiso 1 1 calc R . .  
C34 C 0.8445(7) 0.3841(3) 0.3950(5) 0.025(2) Uani 1 1 d . . .  
H34 H 0.8806 0.3804 0.4453 0.030 Uiso 1 1 calc R . .  
C35 C 0.7775(6) 0.4276(3) 0.3796(5) 0.0160(17) Uani 1 1 d . . .  
H35 H 0.7677 0.4535 0.4200 0.019 Uiso 1 1 calc R . .  
C36 C 0.5487(6) 0.4821(3) 0.3439(4) 0.0119(16) Uani 1 1 d . . .  
H36 H 0.5748 0.4772 0.4001 0.014 Uiso 1 1 calc R . .  
C37 C 0.4729(6) 0.4357(3) 0.3246(4) 0.0144(17) Uani 1 1 d . . .

C38 C 0.4152(6) 0.4342(3) 0.2530(4) 0.0162(17) Uani 1 1 d . . .  
H38 H 0.4178 0.4641 0.2185 0.019 Uiso 1 1 calc R . . .  
C39 C 0.3545(6) 0.3904(3) 0.2308(5) 0.0212(19) Uani 1 1 d . . .  
H39 H 0.3164 0.3903 0.1810 0.025 Uiso 1 1 calc R . . .  
C40 C 0.3482(6) 0.3464(3) 0.2800(5) 0.0214(18) Uani 1 1 d . . .  
H40 H 0.3056 0.3161 0.2650 0.026 Uiso 1 1 calc R . . .  
C41 C 0.4072(7) 0.3478(4) 0.3540(5) 0.025(2) Uani 1 1 d . . .  
H41 H 0.4044 0.3182 0.3891 0.030 Uiso 1 1 calc R . . .  
C42 C 0.4679(6) 0.3917(3) 0.3743(4) 0.0148(16) Uani 1 1 d . . .  
H42 H 0.5075 0.3921 0.4235 0.018 Uiso 1 1 calc R . . .  
Co2 Co 0.11574(8) 0.50421(5) 0.82055(6) 0.0076(2) Uani 1 1 d . . .  
N7 N 0.0770(4) 0.5046(3) 0.9342(3) 0.0102(4) Uani 1 1 d U . . .  
H7A H 0.0717 0.5392 0.9519 0.012 Uiso 1 1 calc R . . .  
H7B H 0.0093 0.4885 0.9406 0.012 Uiso 1 1 calc R . . .  
N8 N 0.2186(5) 0.4472(2) 0.8511(3) 0.0108(12) Uani 1 1 d U . . .  
H8A H 0.2130 0.4198 0.8151 0.013 Uiso 1 1 calc R . . .  
H8B H 0.2900 0.4600 0.8503 0.013 Uiso 1 1 calc R . . .  
N9 N 0.0005(5) 0.4519(2) 0.7956(3) 0.0102(13) Uani 1 1 d . . .  
H9A H -0.0007 0.4265 0.8350 0.012 Uiso 1 1 calc R . . .  
H9B H -0.0673 0.4686 0.7944 0.012 Uiso 1 1 calc R . . .  
N10 N 0.1517(4) 0.4973(3) 0.7084(3) 0.0102(4) Uani 1 1 d . . .  
H10A H 0.1627 0.5306 0.6871 0.012 Uiso 1 1 calc R . . .  
H10B H 0.2163 0.4783 0.7037 0.012 Uiso 1 1 calc R . . .  
N11 N 0.0152(5) 0.5644(3) 0.7979(4) 0.0155(14) Uani 1 1 d . . .  
H11A H -0.0262 0.5570 0.7529 0.019 Uiso 1 1 calc R . . .  
H11B H -0.0327 0.5684 0.8395 0.019 Uiso 1 1 calc R . . .  
N12 N 0.2281(5) 0.5599(2) 0.8362(3) 0.0101(13) Uani 1 1 d . . .  
H12A H 0.2675 0.5530 0.8823 0.012 Uiso 1 1 calc R . . .  
H12B H 0.2767 0.5589 0.7947 0.012 Uiso 1 1 calc R . . .  
C43 C 0.1635(6) 0.4755(3) 0.9822(4) 0.0107(12) Uani 1 1 d U . . .  
H43 H 0.2301 0.4988 0.9887 0.013 Uiso 1 1 calc R . . .  
C44 C 0.1215(6) 0.4604(3) 1.0638(4) 0.0113(12) Uani 1 1 d U . . .  
C45 C 0.1626(6) 0.4878(3) 1.1314(4) 0.0106(14) Uani 1 1 d U . . .  
H45 H 0.2156 0.5154 1.1255 0.013 Uiso 1 1 calc R . . .  
C46 C 0.1260(6) 0.4745(3) 1.2049(5) 0.0180(17) Uani 1 1 d . . .  
H46 H 0.1532 0.4935 1.2499 0.022 Uiso 1 1 calc R . . .  
C47 C 0.0500(6) 0.4339(3) 1.2155(4) 0.0184(18) Uani 1 1 d . . .  
H47 H 0.0266 0.4246 1.2674 0.022 Uiso 1 1 calc R . . .  
C48 C 0.0087(6) 0.4071(3) 1.1495(4) 0.0151(15) Uani 1 1 d U . . .  
H48 H -0.0442 0.3795 1.1562 0.018 Uiso 1 1 calc R . . .  
C49 C 0.0434(6) 0.4200(3) 1.0743(4) 0.0139(13) Uani 1 1 d U . . .  
H49 H 0.0142 0.4014 1.0295 0.017 Uiso 1 1 calc R . . .  
C50 C 0.1939(5) 0.4267(3) 0.9330(4) 0.0093(11) Uani 1 1 d U . . .  
H50 H 0.1265 0.4036 0.9285 0.011 Uiso 1 1 calc R . . .  
C51 C 0.2849(5) 0.3937(3) 0.9701(4) 0.0102(4) Uani 1 1 d U . . .  
C52 C 0.3915(6) 0.4154(3) 0.9827(4) 0.0157(14) Uani 1 1 d U . . .

H52 H 0.4079 0.4506 0.9657 0.019 Uiso 1 1 calc R ..  
C53 C 0.4719(7) 0.3848(4) 1.0203(6) 0.029(2) Uani 1 1 d ...  
H53 H 0.5422 0.3998 1.0325 0.035 Uiso 1 1 calc R ..  
C54 C 0.4507(7) 0.3338(4) 1.0395(5) 0.028(2) Uani 1 1 d ...  
H54 H 0.5089 0.3121 1.0599 0.034 Uiso 1 1 calc R ..  
C55 C 0.3495(7) 0.3131(3) 1.0304(6) 0.029(2) Uani 1 1 d ...  
H55 H 0.3348 0.2778 1.0480 0.035 Uiso 1 1 calc R ..  
C56 C 0.2658(6) 0.3433(3) 0.9949(4) 0.0164(14) Uani 1 1 d U ..  
H56 H 0.1941 0.3283 0.9881 0.020 Uiso 1 1 calc R ..  
C57 C 0.0194(6) 0.4257(3) 0.7178(4) 0.0088(15) Uani 1 1 d ...  
H57 H 0.0795 0.3987 0.7250 0.011 Uiso 1 1 calc R ..  
C58 C -0.0808(6) 0.3982(3) 0.6845(4) 0.0102(4) Uani 1 1 d ...  
C59 C -0.0700(8) 0.3530(4) 0.6413(6) 0.035(2) Uani 1 1 d ...  
H59 H 0.0013 0.3378 0.6348 0.042 Uiso 1 1 calc R ..  
C60 C -0.1636(8) 0.3279(4) 0.6054(5) 0.039(3) Uani 1 1 d ...  
H60 H -0.1557 0.2958 0.5760 0.047 Uiso 1 1 calc R ..  
C61 C -0.2642(8) 0.3506(5) 0.6141(5) 0.039(3) Uani 1 1 d ...  
H61 H -0.3270 0.3338 0.5903 0.047 Uiso 1 1 calc R ..  
C62 C -0.2787(7) 0.3964(4) 0.6556(6) 0.035(2) Uani 1 1 d ...  
H62 H -0.3507 0.4111 0.6603 0.042 Uiso 1 1 calc R ..  
C63 C -0.1889(7) 0.4218(3) 0.6910(5) 0.028(2) Uani 1 1 d ...  
H63 H -0.1985 0.4543 0.7192 0.033 Uiso 1 1 calc R ..  
C64 C 0.0611(5) 0.4697(3) 0.6630(4) 0.0100(15) Uani 1 1 d ...  
H64 H -0.0005 0.4958 0.6548 0.012 Uiso 1 1 calc R ..  
C65 C 0.0980(6) 0.4512(3) 0.5819(4) 0.0120(13) Uani 1 1 d U ..  
C66 C 0.1829(6) 0.4154(3) 0.5736(4) 0.0178(15) Uani 1 1 d U ..  
H66 H 0.2205 0.4022 0.6195 0.021 Uiso 1 1 calc R ..  
C67 C 0.2143(7) 0.3984(4) 0.4990(5) 0.029(2) Uani 1 1 d ...  
H67 H 0.2696 0.3718 0.4941 0.035 Uiso 1 1 calc R ..  
C68 C 0.1651(6) 0.4204(4) 0.4307(4) 0.0199(18) Uani 1 1 d ...  
H68 H 0.1902 0.4113 0.3792 0.024 Uiso 1 1 calc R ..  
C69 C 0.0785(7) 0.4558(3) 0.4407(4) 0.0185(18) Uani 1 1 d ...  
H69 H 0.0414 0.4695 0.3949 0.022 Uiso 1 1 calc R ..  
C70 C 0.0444(6) 0.4721(3) 0.5146(4) 0.0113(14) Uani 1 1 d U ..  
H70 H -0.0144 0.4969 0.5198 0.014 Uiso 1 1 calc R ..  
C71 C 0.0763(5) 0.6154(3) 0.7860(4) 0.0109(13) Uani 1 1 d U ..  
H71 H 0.1016 0.6167 0.7297 0.013 Uiso 1 1 calc R ..  
C72 C 0.0064(6) 0.6641(3) 0.8016(4) 0.0102(4) Uani 1 1 d U ..  
C73 C 0.0073(6) 0.7071(3) 0.7486(5) 0.0150(14) Uani 1 1 d U ..  
H73 H 0.0468 0.7044 0.7003 0.018 Uiso 1 1 calc R ..  
C74 C -0.0482(7) 0.7527(3) 0.7658(5) 0.026(2) Uani 1 1 d ...  
H74 H -0.0474 0.7811 0.7285 0.031 Uiso 1 1 calc R ..  
C75 C -0.1064(7) 0.7593(3) 0.8363(5) 0.0214(18) Uani 1 1 d ...  
H75 H -0.1431 0.7917 0.8481 0.026 Uiso 1 1 calc R ..  
C76 C -0.1081(6) 0.7163(3) 0.8884(5) 0.0215(19) Uani 1 1 d ...  
H76 H -0.1478 0.7194 0.9364 0.026 Uiso 1 1 calc R ..

C77 C -0.0535(6) 0.6693(3) 0.8722(4) 0.0155(14) Uani 1 1 d U ..  
H77 H -0.0565 0.6404 0.9087 0.019 Uiso 1 1 calc R ..  
C78 C 0.1788(6) 0.6141(3) 0.8410(4) 0.0139(16) Uani 1 1 d ...  
H78 H 0.1533 0.6195 0.8967 0.017 Uiso 1 1 calc R ..  
C79 C 0.2576(6) 0.6586(3) 0.8220(4) 0.0123(13) Uani 1 1 d U ..  
C80 C 0.3225(6) 0.6565(3) 0.7542(5) 0.0151(15) Uani 1 1 d U ..  
H80 H 0.3223 0.6256 0.7216 0.018 Uiso 1 1 calc R ..  
C81 C 0.3880(6) 0.7006(3) 0.7347(5) 0.0197(18) Uani 1 1 d ...  
H81 H 0.4334 0.6988 0.6892 0.024 Uiso 1 1 calc R ..  
C82 C 0.3882(6) 0.7452(3) 0.7788(5) 0.0229(19) Uani 1 1 d ...  
H82 H 0.4312 0.7751 0.7633 0.028 Uiso 1 1 calc R ..  
C83 C 0.3256(6) 0.7477(3) 0.8468(5) 0.0203(19) Uani 1 1 d ...  
H83 H 0.3278 0.7786 0.8793 0.024 Uiso 1 1 calc R ..  
C84 C 0.2589(6) 0.7046(3) 0.8680(4) 0.0132(14) Uani 1 1 d U ..  
H84 H 0.2144 0.7067 0.9139 0.016 Uiso 1 1 calc R ..  
Cl1 Cl 0.30797(13) 0.60521(8) 0.23378(10) 0.0184(4) Uani 1 1 d ...  
Cl2 Cl 0.80900(15) 0.51614(8) 0.88516(12) 0.0254(5) Uani 1 1 d ...  
Cl3 Cl 0.76984(16) 0.35723(9) 0.02850(12) 0.0261(5) Uani 1 1 d ...  
Cl4 Cl 0.2371(2) 0.26182(9) 0.61770(14) 0.0395(6) Uani 1 1 d ...  
Cl5 Cl 0.41487(15) 0.49961(9) 0.73483(11) 0.0249(5) Uani 1 1 d ...  
Cl6 Cl 0.91871(13) 0.58562(8) 0.39940(10) 0.0162(4) Uani 1 1 d ...  
O1 O 0.0543(5) 0.5982(2) 0.0239(3) 0.0330(15) Uani 1 1 d ...  
H1C H 0.0023 0.5940 0.0568 0.049 Uiso 1 1 d R ..  
H1D H 0.0370 0.6228 -0.0088 0.049 Uiso 1 1 d R ..  
O2 O 0.9435(4) 0.3633(2) 0.8944(3) 0.0220(12) Uani 1 1 d ...  
H2C H 1.0099 0.3745 0.8973 0.033 Uiso 1 1 d R ..  
H2D H 0.9333 0.3471 0.8505 0.033 Uiso 1 1 d R ..  
O3 O 0.7798(6) 0.3064(3) 0.8070(4) 0.054(2) Uani 1 1 d ...  
H3C H 0.7261 0.2876 0.7897 0.081 Uiso 1 1 d R ..  
H3D H 0.7564 0.3283 0.8415 0.081 Uiso 1 1 d R ..  
O4 O 0.2570(5) 0.3501(3) 0.7626(3) 0.0335(15) Uani 1 1 d ...  
H4C H 0.2730 0.3238 0.7333 0.050 Uiso 1 1 d R ..  
H4D H 0.1964 0.3441 0.7859 0.050 Uiso 1 1 d R ..  
O5 O 0.4859(14) 0.3855(6) 0.7689(9) 0.029(4) Uani 0.37 1 d P ..  
H5C H 0.4982 0.3667 0.7264 0.044 Uiso 0.37 1 d PR ..  
H5D H 0.4790 0.4189 0.7560 0.044 Uiso 0.37 1 d PR ..  
O6 O 0.6594(9) 0.3938(3) 0.8602(5) 0.080(3) Uani 1 1 d ...  
H6C H 0.6118 0.3898 0.8230 0.120 Uiso 1 1 d R ..  
H6D H 0.6325 0.3831 0.9038 0.120 Uiso 1 1 d R ..  
O7 O 0.4670(10) 0.3178(6) 0.8364(7) 0.062(4) Uani 0.63 1 d P ..  
H7C H 0.4361 0.2906 0.8590 0.094 Uiso 0.63 1 d PR ..  
H7D H 0.4327 0.3247 0.7917 0.094 Uiso 0.63 1 d PR ..  
O8 O 0.4419(6) 0.3429(3) 0.6015(4) 0.054(2) Uani 1 1 d ...  
H8C H 0.4446 0.3244 0.5592 0.081 Uiso 1 1 d R ..  
H8D H 0.4699 0.3253 0.6400 0.081 Uiso 1 1 d R ..  
O9 O 0.2282(6) 0.7206(3) 0.2980(4) 0.0471(19) Uani 1 1 d ...

H9C H 0.1816 0.7196 0.3352 0.071 Uiso 1 1 d R ..  
H9D H 0.2463 0.6890 0.2853 0.071 Uiso 1 1 d R ..  
O10 O 1.0151(6) 0.7088(3) 0.3807(4) 0.053(2) Uani 1 1 d ...  
H10C H 0.9666 0.7286 0.3584 0.079 Uiso 1 1 d R ..  
H10D H 1.0015 0.6764 0.3698 0.079 Uiso 1 1 d R ..  
O11 O 0.9605(6) 0.7381(3) 0.5363(5) 0.057(2) Uani 1 1 d ...  
H11C H 0.9601 0.7052 0.5481 0.085 Uiso 1 1 d R ..  
H11D H 0.9482 0.7418 0.4867 0.085 Uiso 1 1 d R ..  
O12 O 0.5290(9) 0.2511(4) 0.7228(8) 0.116(5) Uani 1 1 d ...  
H12C H 0.4704 0.2328 0.7276 0.173 Uiso 1 1 d R ..  
H12D H 0.5244 0.2792 0.7509 0.173 Uiso 1 1 d R ..  
O13 O 0.3002(5) 0.7515(2) 0.0631(4) 0.0313(15) Uani 1 1 d ...  
H13A H 0.2870 0.7183 0.0609 0.047 Uiso 1 1 d R ..  
H13B H 0.2750 0.7665 0.0213 0.047 Uiso 1 1 d R ..  
O14 O 0.2626(5) 0.6424(2) 0.0576(3) 0.0268(14) Uani 1 1 d ...  
H14A H 0.1994 0.6290 0.0472 0.040 Uiso 1 1 d R ..  
H14B H 0.2751 0.6324 0.1052 0.040 Uiso 1 1 d R ..  
O15 O 0.3821(4) 0.5619(2) 0.9788(3) 0.0229(13) Uani 1 1 d ...  
H15A H 0.4256 0.5384 0.9606 0.034 Uiso 1 1 d R ..  
H15B H 0.3560 0.5513 1.0226 0.034 Uiso 1 1 d R ..  
O16 O 0.5492(6) 0.5181(5) 0.8899(4) 0.095(4) Uani 1 1 d ...  
H16A H 0.5108 0.5277 0.8496 0.142 Uiso 1 1 d R ..  
H16B H 0.6094 0.5043 0.8745 0.142 Uiso 1 1 d R ..  
O17 O 0.1967(5) 0.5819(2) 0.6055(3) 0.0260(13) Uani 1 1 d ...  
H17A H 0.2437 0.5701 0.5728 0.039 Uiso 1 1 d R ..  
H17B H 0.2152 0.6132 0.6202 0.039 Uiso 1 1 d R ..  
O18 O 0.9788(5) 0.6274(3) 0.5680(4) 0.0355(16) Uani 1 1 d ...  
H18A H 0.9622 0.6161 0.5217 0.053 Uiso 1 1 d R ..  
H18B H 1.0421 0.6144 0.5791 0.053 Uiso 1 1 d R ..  
O19 O 0.8616(5) 0.5280(3) 0.1662(3) 0.0302(15) Uani 1 1 d ...  
H19A H 0.8903 0.4980 0.1549 0.045 Uiso 1 1 d R ..  
H19B H 0.8944 0.5525 0.1410 0.045 Uiso 1 1 d R ..  
O20 O 0.7342(4) 0.4761(3) 0.0525(3) 0.0283(14) Uani 1 1 d ...  
H20A H 0.7608 0.4954 0.0160 0.042 Uiso 1 1 d R ..  
H20B H 0.7620 0.4854 0.0971 0.042 Uiso 1 1 d R ..  
O21 O 0.5270(4) 0.5124(2) 0.1061(3) 0.0172(12) Uani 1 1 d ...  
H21A H 0.4916 0.5271 0.0680 0.026 Uiso 1 1 d R ..  
H21B H 0.5142 0.4791 0.1058 0.026 Uiso 1 1 d R ..  
O22 O 0.1809(5) 0.5666(3) 0.3850(4) 0.0368(16) Uani 1 1 d ...  
H22A H 0.2010 0.5852 0.3455 0.055 Uiso 1 1 d R ..  
H22B H 0.1298 0.5828 0.4092 0.055 Uiso 1 1 d R ..  
O23 O 0.3498(5) 0.5311(2) 0.4801(3) 0.0253(13) Uani 1 1 d ...  
H23A H 0.3663 0.4992 0.4924 0.038 Uiso 1 1 d R ..  
H23B H 0.3004 0.5310 0.4435 0.038 Uiso 1 1 d R ..  
O24 O 0.8516(4) 0.5591(2) 0.6596(3) 0.0259(13) Uani 1 1 d ...  
H24A H 0.8905 0.5799 0.6316 0.039 Uiso 1 1 d R ..

H24B H 0.8213 0.5321 0.6378 0.039 Uiso 1 1 d R . .  
 O25 O 0.6786(5) 0.4986(3) 0.5334(3) 0.0383(17) Uani 1 1 d . . .  
 H25A H 0.7185 0.4971 0.5754 0.057 Uiso 1 1 d R . .  
 H25B H 0.6172 0.4832 0.5415 0.057 Uiso 1 1 d R . .  
 O26 O 0.4723(5) 0.4522(3) 0.5706(3) 0.0310(15) Uani 1 1 d . . .  
 H26A H 0.4632 0.4191 0.5795 0.046 Uiso 1 1 d R . .  
 H26B H 0.4567 0.4653 0.6156 0.046 Uiso 1 1 d R . .

loop\_  
 \_atom\_site\_aniso\_label  
 \_atom\_site\_aniso\_U\_11  
 \_atom\_site\_aniso\_U\_22  
 \_atom\_site\_aniso\_U\_33  
 \_atom\_site\_aniso\_U\_23  
 \_atom\_site\_aniso\_U\_13  
 \_atom\_site\_aniso\_U\_12  
 Co1 0.0025(5) 0.0166(6) 0.0027(5) 0.0007(5) -0.0016(4) 0.0009(5)  
 N1 0.0062(7) 0.0173(8) 0.0068(7) 0.0032(7) -0.0037(6) -0.0007(7)  
 N2 0.004(3) 0.009(3) 0.014(3) -0.002(2) -0.003(2) 0.004(2)  
 N3 0.0062(7) 0.0173(8) 0.0068(7) 0.0032(7) -0.0037(6) -0.0007(7)  
 N4 0.003(3) 0.023(4) 0.011(3) 0.001(3) -0.004(2) 0.002(3)  
 N5 0.0062(7) 0.0173(8) 0.0068(7) 0.0032(7) -0.0037(6) -0.0007(7)  
 N6 0.0062(7) 0.0173(8) 0.0068(7) 0.0032(7) -0.0037(6) -0.0007(7)  
 C1 0.008(2) 0.022(3) 0.001(2) -0.003(2) -0.001(2) -0.004(2)  
 C2 0.008(2) 0.027(3) 0.006(2) -0.003(2) 0.003(2) -0.001(2)  
 C3 0.008(3) 0.029(4) 0.009(3) 0.001(3) 0.004(2) -0.004(3)  
 C4 0.018(4) 0.040(5) 0.006(4) -0.005(3) 0.004(3) 0.001(4)  
 C5 0.011(4) 0.033(5) 0.010(4) -0.008(3) 0.002(3) 0.009(3)  
 C6 0.017(3) 0.038(4) 0.011(3) -0.005(3) -0.006(3) -0.003(3)  
 C7 0.014(3) 0.033(3) 0.011(3) 0.001(3) 0.002(2) -0.001(3)  
 C8 0.011(3) 0.019(3) 0.004(3) -0.003(2) 0.002(2) -0.003(2)  
 C9 0.014(3) 0.013(3) 0.010(3) -0.001(2) 0.005(2) -0.002(2)  
 C10 0.019(3) 0.018(4) 0.025(4) -0.003(3) 0.011(3) -0.001(3)  
 C11 0.015(4) 0.021(5) 0.042(5) 0.011(4) 0.012(4) 0.001(3)  
 C12 0.045(6) 0.034(6) 0.015(4) 0.004(4) 0.017(4) 0.014(4)  
 C13 0.039(5) 0.015(4) 0.017(4) -0.009(3) -0.007(4) 0.021(4)  
 C14 0.021(4) 0.032(5) 0.016(4) 0.002(4) -0.007(3) 0.000(4)  
 C15 0.0062(7) 0.0173(8) 0.0068(7) 0.0032(7) -0.0037(6) -0.0007(7)  
 C16 0.007(3) 0.012(4) 0.008(4) 0.001(3) -0.006(3) 0.001(3)  
 C17 0.003(4) 0.024(5) 0.055(6) 0.005(4) -0.004(4) -0.001(3)  
 C18 0.019(5) 0.047(7) 0.059(7) 0.031(5) -0.010(4) -0.016(4)  
 C19 0.015(4) 0.037(6) 0.042(6) -0.004(4) -0.004(4) -0.014(4)  
 C20 0.013(4) 0.035(5) 0.013(4) -0.002(4) 0.000(3) 0.009(4)  
 C21 0.022(4) 0.029(5) 0.010(4) 0.002(3) -0.002(3) 0.001(4)  
 C22 0.0062(7) 0.0173(8) 0.0068(7) 0.0032(7) -0.0037(6) -0.0007(7)  
 C23 0.004(3) 0.011(4) 0.009(4) 0.004(3) -0.002(3) -0.001(3)

C24 0.012(3) 0.019(3) 0.008(3) 0.006(3) -0.001(3) 0.003(3)  
 C25 0.0062(7) 0.0173(8) 0.0068(7) 0.0032(7) -0.0037(6) -0.0007(7)  
 C26 0.013(4) 0.037(5) 0.003(4) 0.003(3) -0.004(3) -0.006(3)  
 C27 0.016(4) 0.029(5) 0.015(4) 0.003(3) 0.009(3) 0.011(3)  
 C28 0.011(4) 0.028(5) 0.006(4) 0.004(3) 0.001(3) -0.003(3)  
 C29 0.009(3) 0.011(3) 0.010(3) 0.002(2) -0.003(2) -0.005(2)  
 C30 0.017(3) 0.014(3) 0.013(3) -0.004(3) 0.012(3) -0.006(3)  
 C31 0.023(3) 0.020(3) 0.018(3) -0.002(3) 0.013(3) -0.004(3)  
 C32 0.027(3) 0.018(3) 0.028(3) -0.004(3) 0.021(3) -0.005(3)  
 C33 0.028(4) 0.014(4) 0.035(4) 0.007(3) 0.021(3) 0.001(3)  
 C34 0.017(4) 0.030(5) 0.028(5) 0.008(4) 0.006(4) 0.010(4)  
 C35 0.013(4) 0.019(4) 0.015(4) 0.002(3) -0.004(3) 0.002(3)  
 C36 0.014(4) 0.016(4) 0.005(4) -0.001(3) -0.005(3) 0.000(3)  
 C37 0.003(3) 0.030(5) 0.010(4) 0.000(3) 0.002(3) 0.000(3)  
 C38 0.012(4) 0.024(5) 0.012(4) 0.007(3) -0.007(3) -0.005(3)  
 C39 0.012(4) 0.034(5) 0.017(4) -0.003(4) -0.007(3) -0.011(4)  
 C40 0.017(4) 0.025(5) 0.022(5) -0.006(4) 0.004(3) -0.002(3)  
 C41 0.035(5) 0.025(5) 0.016(4) 0.006(4) 0.008(4) -0.005(4)  
 C42 0.013(4) 0.023(5) 0.009(4) -0.004(3) -0.004(3) -0.001(3)  
 Co2 0.0027(5) 0.0167(7) 0.0033(5) 0.0025(5) -0.0012(4) -0.0001(5)  
 N7 0.0062(7) 0.0173(8) 0.0068(7) 0.0032(7) -0.0037(6) -0.0007(7)  
 N8 0.006(3) 0.021(3) 0.005(3) 0.000(2) -0.001(2) 0.001(2)  
 N9 0.006(3) 0.017(3) 0.007(3) 0.001(2) -0.002(2) 0.002(2)  
 N10 0.0062(7) 0.0173(8) 0.0068(7) 0.0032(7) -0.0037(6) -0.0007(7)  
 N11 0.006(3) 0.036(4) 0.004(3) 0.004(3) 0.001(2) -0.005(3)  
 N12 0.011(3) 0.017(3) 0.002(3) 0.002(2) -0.002(2) -0.001(3)  
 C43 0.006(2) 0.018(3) 0.008(2) 0.004(2) -0.004(2) -0.001(2)  
 C44 0.009(2) 0.017(3) 0.008(2) 0.002(2) -0.005(2) -0.002(2)  
 C45 0.009(3) 0.015(3) 0.007(3) -0.004(3) -0.005(2) 0.001(3)  
 C46 0.023(4) 0.020(5) 0.010(4) -0.004(3) -0.005(3) -0.002(3)  
 C47 0.020(4) 0.027(5) 0.008(4) 0.006(3) -0.004(3) 0.004(3)  
 C48 0.013(3) 0.021(4) 0.012(3) 0.005(3) -0.002(3) -0.006(3)  
 C49 0.015(3) 0.020(3) 0.008(3) 0.002(2) -0.003(2) -0.006(2)  
 C50 0.006(2) 0.016(3) 0.006(2) 0.003(2) -0.002(2) -0.001(2)  
 C51 0.0062(7) 0.0173(8) 0.0068(7) 0.0032(7) -0.0037(6) -0.0007(7)  
 C52 0.010(3) 0.017(3) 0.020(3) 0.002(3) -0.004(3) -0.002(3)  
 C53 0.011(4) 0.028(5) 0.047(6) -0.016(4) -0.013(4) 0.008(4)  
 C54 0.017(4) 0.033(6) 0.034(5) 0.003(4) -0.009(4) 0.017(4)  
 C55 0.033(5) 0.010(5) 0.045(6) 0.002(4) 0.005(4) 0.008(4)  
 C56 0.010(3) 0.023(3) 0.015(3) 0.003(3) -0.005(3) 0.001(3)  
 C57 0.010(3) 0.009(4) 0.008(4) 0.003(3) 0.004(3) -0.001(3)  
 C58 0.0062(7) 0.0173(8) 0.0068(7) 0.0032(7) -0.0037(6) -0.0007(7)  
 C59 0.032(5) 0.028(5) 0.046(6) -0.014(4) 0.004(4) -0.016(4)  
 C60 0.048(6) 0.053(7) 0.016(5) -0.012(4) -0.003(4) -0.005(5)  
 C61 0.032(5) 0.072(8) 0.012(5) 0.000(5) -0.009(4) -0.020(5)  
 C62 0.020(5) 0.033(6) 0.051(6) 0.011(5) -0.015(4) -0.017(4)

C63 0.034(5) 0.011(4) 0.038(5) -0.002(4) -0.007(4) -0.001(4)  
 C64 0.002(3) 0.023(4) 0.006(4) 0.000(3) 0.000(3) -0.002(3)  
 C65 0.008(3) 0.022(3) 0.005(3) 0.005(2) -0.004(2) -0.006(2)  
 C66 0.012(3) 0.034(4) 0.008(3) 0.007(3) -0.004(3) 0.001(3)  
 C67 0.023(4) 0.053(6) 0.012(4) 0.002(4) 0.003(3) 0.022(4)  
 C68 0.019(4) 0.037(5) 0.004(4) 0.001(3) 0.002(3) 0.007(4)  
 C69 0.026(4) 0.020(5) 0.009(4) 0.000(3) -0.014(3) 0.001(3)  
 C70 0.010(3) 0.014(3) 0.009(3) 0.003(3) -0.007(3) -0.005(3)  
 C71 0.007(3) 0.017(3) 0.008(3) 0.000(3) -0.001(2) -0.001(2)  
 C72 0.0062(7) 0.0173(8) 0.0068(7) 0.0032(7) -0.0037(6) -0.0007(7)  
 C73 0.010(3) 0.017(3) 0.018(3) 0.004(3) 0.001(3) 0.000(3)  
 C74 0.025(5) 0.016(5) 0.036(5) 0.004(4) -0.003(4) 0.000(4)  
 C75 0.020(4) 0.011(4) 0.033(5) -0.007(4) -0.002(4) 0.005(3)  
 C76 0.015(4) 0.032(5) 0.018(4) -0.005(4) -0.002(3) -0.001(4)  
 C77 0.015(3) 0.019(3) 0.013(3) 0.004(3) -0.002(3) 0.005(3)  
 C78 0.013(4) 0.021(4) 0.007(4) 0.002(3) -0.001(3) 0.000(3)  
 C79 0.008(3) 0.009(3) 0.019(3) 0.006(2) -0.004(2) -0.001(2)  
 C80 0.007(3) 0.015(3) 0.023(3) 0.007(3) -0.004(3) 0.002(3)  
 C81 0.018(4) 0.007(4) 0.034(5) 0.010(4) 0.012(4) 0.004(3)  
 C82 0.012(4) 0.025(5) 0.032(5) 0.003(4) -0.010(4) -0.006(3)  
 C83 0.019(4) 0.016(5) 0.025(5) 0.006(3) -0.015(4) -0.004(3)  
 C84 0.010(3) 0.012(3) 0.018(3) -0.002(3) -0.004(3) 0.001(3)  
 CI1 0.0067(8) 0.0337(12) 0.0146(9) 0.0006(8) -0.0048(7) 0.0010(7)  
 CI2 0.0144(9) 0.0356(13) 0.0265(11) 0.0072(9) 0.0101(8) 0.0066(8)  
 CI3 0.0216(10) 0.0296(12) 0.0269(11) 0.0047(9) -0.0052(8) -0.0059(9)  
 CI4 0.0680(17) 0.0167(11) 0.0343(13) 0.0041(9) 0.0136(11) 0.0115(11)  
 CI5 0.0137(9) 0.0407(13) 0.0203(10) -0.0063(9) 0.0003(7) -0.0031(9)  
 CI6 0.0098(8) 0.0223(10) 0.0162(9) 0.0016(8) -0.0068(7) 0.0033(7)  
 O1 0.054(4) 0.028(4) 0.016(3) -0.006(3) -0.011(3) 0.011(3)  
 O2 0.024(3) 0.022(3) 0.020(3) 0.000(2) 0.002(2) -0.010(2)  
 O3 0.058(5) 0.065(6) 0.039(4) 0.002(4) -0.001(4) -0.002(4)  
 O4 0.033(4) 0.042(4) 0.025(3) -0.005(3) -0.003(3) 0.009(3)  
 O5 0.047(10) 0.021(9) 0.020(9) 0.003(7) 0.000(7) -0.003(7)  
 O6 0.150(9) 0.039(5) 0.050(5) -0.007(4) -0.047(6) 0.032(5)  
 O7 0.065(8) 0.093(10) 0.029(6) -0.024(6) -0.018(6) 0.054(8)  
 O8 0.055(5) 0.080(6) 0.027(4) 0.012(4) 0.004(3) 0.024(4)  
 O9 0.045(4) 0.063(5) 0.033(4) -0.002(3) -0.005(3) 0.010(4)  
 O10 0.060(5) 0.055(5) 0.042(4) 0.005(4) -0.009(4) -0.005(4)  
 O11 0.054(5) 0.063(6) 0.054(5) -0.005(4) 0.024(4) -0.011(4)  
 O12 0.083(7) 0.095(9) 0.166(12) -0.081(8) -0.069(7) 0.029(6)  
 O13 0.029(3) 0.025(4) 0.040(4) 0.004(3) 0.006(3) 0.006(3)  
 O14 0.029(3) 0.037(4) 0.014(3) 0.010(3) 0.002(2) 0.001(3)  
 O15 0.020(3) 0.033(3) 0.015(3) 0.001(2) -0.006(2) -0.006(2)  
 O16 0.033(4) 0.222(13) 0.030(4) 0.000(6) 0.001(3) -0.049(6)  
 O17 0.051(4) 0.014(3) 0.014(3) 0.001(2) 0.011(3) -0.008(3)  
 O18 0.022(3) 0.060(5) 0.025(3) -0.014(3) 0.001(3) -0.005(3)

O19 0.027(3) 0.034(4) 0.029(3) -0.005(3) -0.005(3) 0.015(3)  
O20 0.022(3) 0.049(4) 0.014(3) 0.002(3) -0.002(2) -0.011(3)  
O21 0.033(3) 0.011(3) 0.007(2) 0.004(2) -0.007(2) -0.008(2)  
O22 0.019(3) 0.055(5) 0.036(4) 0.020(3) 0.001(3) -0.006(3)  
O23 0.028(3) 0.030(4) 0.018(3) 0.001(2) 0.001(2) -0.009(3)  
O24 0.017(3) 0.036(4) 0.025(3) 0.001(3) 0.000(2) 0.008(3)  
O25 0.039(4) 0.057(5) 0.019(3) -0.005(3) -0.002(3) 0.025(3)  
O26 0.026(3) 0.044(4) 0.022(3) -0.003(3) -0.002(3) 0.002(3)

\_geom\_special\_details

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All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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loop\_

\_geom\_bond\_atom\_site\_label\_1  
\_geom\_bond\_atom\_site\_label\_2  
\_geom\_bond\_distance  
\_geom\_bond\_site\_symmetry\_2  
\_geom\_bond\_publ\_flag

Co1 N1 1.949(5) . ?

Co1 N4 1.954(5) . ?

Co1 N3 1.958(6) . ?

Co1 N5 1.961(6) . ?

Co1 N2 1.963(6) . ?

Co1 N6 1.967(6) . ?

N1 C1 1.508(9) . ?

N1 H1A 0.9200 . ?

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N2 H2B 0.9200 . ?

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Co2 N8 1.959(6) . ?  
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O1 H1D 0.8501 . ?  
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O2 H2D 0.8506 . ?  
O3 H3C 0.8500 . ?  
O3 H3D 0.8501 . ?  
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O4 H4D 0.8497 . ?  
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O8 H8D 0.8501 . ?  
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O10 H10D 0.8502 . ?  
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H1A N1 H1B 108.0 . . ?  
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C15 N3 H3B 109.0 . . ?  
Co1 N3 H3B 109.0 . . ?  
H3A N3 H3B 107.8 . . ?  
C22 N4 Co1 111.1(4) . . ?  
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Co1 N4 H4A 109.4 . . ?  
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Co1 N4 H4B 109.4 . . ?  
H4A N4 H4B 108.0 . . ?  
C29 N5 Co1 111.9(4) . . ?  
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C29 N5 H5B 109.2 . . ?  
Co1 N5 H5B 109.2 . . ?  
H5A N5 H5B 107.9 . . ?  
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Co1 N6 H6B 109.1 . . ?  
H6A N6 H6B 107.9 . . ?  
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N1 C1 H1 108.0 . . ?  
C8 C1 H1 108.0 . . ?  
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C7 C2 C1 120.7(7) . . ?  
C4 C3 C2 121.2(7) . . ?  
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C2 C3 H3 119.4 . . ?  
C3 C4 C5 121.6(8) . . ?  
C3 C4 H4 119.2 . . ?

C5 C4 H4 119.2 . . ?  
C4 C5 C6 118.9(7) . . ?  
C4 C5 H5 120.5 . . ?  
C6 C5 H5 120.5 . . ?  
C5 C6 C7 119.4(8) . . ?  
C5 C6 H6 120.3 . . ?  
C7 C6 H6 120.3 . . ?  
C2 C7 C6 121.1(7) . . ?  
C2 C7 H7 119.5 . . ?  
C6 C7 H7 119.5 . . ?  
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N2 C8 C1 107.9(6) . . ?  
C9 C8 C1 110.8(6) . . ?  
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C9 C8 H8 108.2 . . ?  
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C14 C9 C10 118.4(7) . . ?  
C14 C9 C8 120.6(7) . . ?  
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C12 C13 C14 120.8(8) . . ?  
C12 C13 H13 119.6 . . ?  
C14 C13 H13 119.6 . . ?  
C13 C14 C9 120.4(8) . . ?  
C13 C14 H14 119.8 . . ?  
C9 C14 H14 119.8 . . ?  
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C16 C15 C22 112.3(6) . . ?  
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C16 C15 H15 108.7 . . ?  
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C21 C16 C15 121.3(7) . . ?  
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C18 C17 H17 119.5 . . ?

C19 C18 C17 119.4(9) . . ?  
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C23 C22 C15 112.6(6) . . ?  
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Co2 N7 H7A 109.6 . . ?  
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Co2 N7 H7B 109.6 . . ?  
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Co2 N8 H8B 109.5 . . ?  
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H9A N9 H9B 108.0 . . ?  
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C48 C47 H47 120.5 . . ?  
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C47 C48 H48 119.6 . . ?  
C48 C49 C44 120.2(7) . . ?  
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C51 C50 N8 114.4(6) . . ?  
C51 C50 C43 113.4(6) . . ?  
N8 C50 C43 105.9(6) . . ?  
C51 C50 H50 107.6 . . ?  
N8 C50 H50 107.6 . . ?  
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C52 C51 C50 120.7(7) . . ?  
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C51 C56 H56 119.5 . . ?  
C55 C56 H56 119.5 . . ?  
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N12 C78 C71 107.8(6) . . ?  
C79 C78 C71 111.3(6) . . ?  
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C83 C84 H84 119.9 . . ?  
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H12C O12 H12D 109.5 . . ?  
H13A O13 H13B 109.5 . . ?  
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H17A O17 H17B 109.5 . . ?  
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H18B O18 H18B 0.0 . . ?  
H18A O18 H18B 105.7 . . ?  
H18A O18 H18B 105.7 . . ?  
H19A O19 H19B 109.5 . . ?  
H20A O20 H20B 109.5 . . ?  
H21A O21 H21B 109.5 . . ?  
H22A O22 H22B 109.4 . . ?  
H23A O23 H23B 109.5 . . ?  
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H24A O24 H24B 119.2 . . ?  
H25A O25 H25B 109.5 . . ?  
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H26B O26 H26A 101.0 . . ?  
H26A O26 H26B 101.0 . . ?  
H26B O26 H26B 0.0 . . ?  
H26A O26 H26B 101.0 . . ?

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N2 Co1 N1 C1 15.1(5) . . . ?  
N6 Co1 N1 C1 -77.4(5) . . . ?  
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N4 Co1 N2 C8 -164.1(5) . . . ?  
N3 Co1 N2 C8 -79.8(5) . . . ?  
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N6 Co1 N2 C8 103.5(5) . . . ?  
N1 Co1 N3 C15 -171.2(5) . . . ?  
N4 Co1 N3 C15 6.6(5) . . . ?  
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N2 Co1 N3 C15 -86.0(5) . . . ?  
N6 Co1 N3 C15 49(3) . . . ?  
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N5 Co1 N4 C22 -72.1(5) . . . ?  
N2 Co1 N4 C22 110.3(5) . . . ?  
N6 Co1 N4 C22 -156.9(5) . . . ?  
N1 Co1 N5 C29 104.2(5) . . . ?  
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N3 Co1 N5 C29 -164.4(5) . . . ?  
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N1 Co1 N6 C36 -79.3(5) . . . ?  
N4 Co1 N6 C36 102.6(5) . . . ?  
N3 Co1 N6 C36 61(3) . . . ?  
N5 Co1 N6 C36 11.5(5) . . . ?  
N2 Co1 N6 C36 -164.6(5) . . . ?  
Co1 N1 C1 C2 -162.9(5) . . . ?  
Co1 N1 C1 C8 -37.4(6) . . . ?  
N1 C1 C2 C3 -107.6(8) . . . ?  
C8 C1 C2 C3 131.5(7) . . . ?

N1 C1 C2 C7 71.0(9) . . . ?  
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C7 C2 C3 C4 1.1(12) . . . ?  
C1 C2 C3 C4 179.8(7) . . . ?  
C2 C3 C4 C5 -0.3(12) . . . ?  
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C1 C2 C7 C6 -179.4(7) . . . ?  
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Co1 N2 C8 C9 -158.4(5) . . . ?  
Co1 N2 C8 C1 -35.2(6) . . . ?  
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N1 C1 C8 N2 46.0(7) . . . ?  
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N1 C1 C8 C9 170.8(6) . . . ?  
N2 C8 C9 C14 -131.8(7) . . . ?  
C1 C8 C9 C14 106.7(8) . . . ?  
N2 C8 C9 C10 51.7(10) . . . ?  
C1 C8 C9 C10 -69.9(9) . . . ?  
C14 C9 C10 C11 0.2(12) . . . ?  
C8 C9 C10 C11 176.8(7) . . . ?  
C9 C10 C11 C12 -1.5(13) . . . ?  
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C12 C13 C14 C9 -3.1(12) . . . ?  
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C8 C9 C14 C13 -174.5(7) . . . ?  
Co1 N3 C15 C16 -153.1(5) . . . ?  
Co1 N3 C15 C22 -30.0(6) . . . ?  
N3 C15 C16 C17 -139.9(7) . . . ?  
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C22 C15 C16 C21 -75.5(8) . . . ?  
C21 C16 C17 C18 -0.2(13) . . . ?  
C15 C16 C17 C18 -176.3(8) . . . ?  
C16 C17 C18 C19 -2.6(16) . . . ?  
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C18 C19 C20 C21 -0.5(14) . . . ?  
C19 C20 C21 C16 -2.4(12) . . . ?  
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C15 C16 C21 C20 178.7(7) . . . ?  
Co1 N4 C22 C23 -166.2(5) . . . ?  
Co1 N4 C22 C15 -41.3(6) . . . ?  
N3 C15 C22 N4 44.9(7) . . . ?  
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N3 C15 C22 C23 170.4(5) . . . ?  
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C28 C23 C24 C25 -1.0(11) . . . ?  
C22 C23 C24 C25 -177.1(6) . . . ?  
C23 C24 C25 C26 0.2(11) . . . ?  
C24 C25 C26 C27 -1.0(11) . . . ?  
C25 C26 C27 C28 2.5(12) . . . ?  
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C22 C23 C28 C27 178.7(7) . . . ?  
C26 C27 C28 C23 -3.4(12) . . . ?  
Co1 N5 C29 C30 -159.2(5) . . . ?  
Co1 N5 C29 C36 -32.5(6) . . . ?  
N5 C29 C30 C31 -122.3(7) . . . ?  
C36 C29 C30 C31 113.5(8) . . . ?  
N5 C29 C30 C35 58.8(9) . . . ?  
C36 C29 C30 C35 -65.5(9) . . . ?  
C35 C30 C31 C32 1.5(11) . . . ?  
C29 C30 C31 C32 -177.5(7) . . . ?  
C30 C31 C32 C33 -2.9(12) . . . ?  
C31 C32 C33 C34 2.5(12) . . . ?  
C32 C33 C34 C35 -0.8(12) . . . ?  
C33 C34 C35 C30 -0.5(12) . . . ?  
C31 C30 C35 C34 0.2(11) . . . ?  
C29 C30 C35 C34 179.2(7) . . . ?  
Co1 N6 C36 C37 -158.1(5) . . . ?  
Co1 N6 C36 C29 -31.7(6) . . . ?  
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N5 C29 C36 C37 169.6(6) . . . ?  
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N6 C36 C37 C38 54.8(9) . . . ?  
C29 C36 C37 C38 -69.7(9) . . . ?  
N6 C36 C37 C42 -131.5(7) . . . ?  
C29 C36 C37 C42 104.0(8) . . . ?  
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C37 C38 C39 C40 0.7(12) . . . ?  
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C39 C40 C41 C42 -0.1(12) . . . ?  
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C38 C37 C42 C41 -0.4(11) . . . ?  
C36 C37 C42 C41 -174.2(7) . . . ?

N10 Co2 N7 C43 68(3) . . . ?  
N9 Co2 N7 C43 106.5(5) . . . ?  
N8 Co2 N7 C43 15.9(5) . . . ?  
N12 Co2 N7 C43 -76.7(5) . . . ?  
N11 Co2 N7 C43 -161.3(5) . . . ?  
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N9 Co2 N8 C50 -78.2(5) . . . ?  
N12 Co2 N8 C50 105.6(5) . . . ?  
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N10 Co2 N9 C57 14.7(5) . . . ?  
N8 Co2 N9 C57 -77.4(5) . . . ?  
N12 Co2 N9 C57 56(3) . . . ?  
N11 Co2 N9 C57 106.1(5) . . . ?  
N7 Co2 N9 C57 -162.2(5) . . . ?  
N9 Co2 N10 C64 14.3(5) . . . ?  
N8 Co2 N10 C64 104.8(5) . . . ?  
N12 Co2 N10 C64 -162.3(5) . . . ?  
N11 Co2 N10 C64 -77.8(5) . . . ?  
N7 Co2 N10 C64 53(3) . . . ?  
N10 Co2 N11 C71 -78.7(5) . . . ?  
N9 Co2 N11 C71 -163.1(5) . . . ?  
N8 Co2 N11 C71 67(3) . . . ?  
N12 Co2 N11 C71 12.8(5) . . . ?  
N7 Co2 N11 C71 105.0(5) . . . ?  
N10 Co2 N12 C78 103.7(5) . . . ?  
N9 Co2 N12 C78 63(3) . . . ?  
N8 Co2 N12 C78 -164.0(5) . . . ?  
N11 Co2 N12 C78 12.3(5) . . . ?  
N7 Co2 N12 C78 -79.1(5) . . . ?  
Co2 N7 C43 C44 -162.8(5) . . . ?  
Co2 N7 C43 C50 -40.8(6) . . . ?  
N7 C43 C44 C49 72.2(9) . . . ?  
C50 C43 C44 C49 -46.1(9) . . . ?  
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C46 C47 C48 C49 0.8(12) . . . ?  
C47 C48 C49 C44 0.3(12) . . . ?  
C45 C44 C49 C48 -0.7(11) . . . ?  
C43 C44 C49 C48 179.1(7) . . . ?  
Co2 N8 C50 C51 -164.7(5) . . . ?  
Co2 N8 C50 C43 -39.1(6) . . . ?

N7 C43 C50 C51 177.0(6) . . . ?  
C44 C43 C50 C51 -61.3(8) . . . ?  
N7 C43 C50 N8 50.8(6) . . . ?  
C44 C43 C50 N8 172.5(5) . . . ?  
N8 C50 C51 C56 -123.3(7) . . . ?  
C43 C50 C51 C56 115.2(8) . . . ?  
N8 C50 C51 C52 59.3(9) . . . ?  
C43 C50 C51 C52 -62.2(9) . . . ?  
C56 C51 C52 C53 -0.4(11) . . . ?  
C50 C51 C52 C53 177.1(7) . . . ?  
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C54 C55 C56 C51 -0.6(13) . . . ?  
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Co2 N9 C57 C64 -39.1(6) . . . ?  
N9 C57 C58 C59 -146.4(8) . . . ?  
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N9 C57 C58 C63 39.7(9) . . . ?  
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C63 C58 C59 C60 -2.4(13) . . . ?  
C57 C58 C59 C60 -176.5(8) . . . ?  
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C60 C61 C62 C63 0.0(15) . . . ?  
C61 C62 C63 C58 -1.3(14) . . . ?  
C59 C58 C63 C62 2.5(12) . . . ?  
C57 C58 C63 C62 176.5(8) . . . ?  
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Co2 N10 C64 C57 -38.8(6) . . . ?  
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C58 C57 C64 N10 173.4(6) . . . ?  
N9 C57 C64 C65 173.8(5) . . . ?  
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N10 C64 C65 C66 60.7(9) . . . ?  
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C64 C65 C66 C67 179.1(8) . . . ?  
C65 C66 C67 C68 4.5(14) . . . ?  
C66 C67 C68 C69 -5.3(14) . . . ?  
C67 C68 C69 C70 3.7(13) . . . ?  
C68 C69 C70 C65 -1.1(12) . . . ?

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Co2 N11 C71 C78 -33.9(6) . . . ?  
N11 C71 C72 C73 -134.5(7) . . . ?  
C78 C71 C72 C73 104.8(7) . . . ?  
N11 C71 C72 C77 50.7(9) . . . ?  
C78 C71 C72 C77 -70.1(8) . . . ?  
C77 C72 C73 C74 0.5(11) . . . ?  
C71 C72 C73 C74 -174.5(7) . . . ?  
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C75 C76 C77 C72 0.5(12) . . . ?  
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N11 C71 C78 C79 168.8(6) . . . ?  
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N12 C78 C79 C84 -137.6(7) . . . ?  
C71 C78 C79 C84 99.9(8) . . . ?  
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C71 C78 C79 C80 -74.1(8) . . . ?  
C84 C79 C80 C81 0.6(10) . . . ?  
C78 C79 C80 C81 174.7(7) . . . ?  
C79 C80 C81 C82 -1.4(12) . . . ?  
C80 C81 C82 C83 2.4(12) . . . ?  
C81 C82 C83 C84 -2.5(11) . . . ?  
C80 C79 C84 C83 -0.8(10) . . . ?  
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C82 C83 C84 C79 1.8(11) . . . ?

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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F^2^, conventional R-factors R are based
on F, with F set to zero for negative F^2^. The threshold expression of
F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F^2^ are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
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loop\_

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 H1A H 0.1377 0.1785 0.7751 0.026 Uiso 1 1 d R . .  
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 N2 N 0.2120(2) -0.0327(2) 0.75287(14) 0.0179(8) Uani 1 1 d . . .  
 H2A H 0.2342 -0.0728 0.7790 0.027 Uiso 1 1 d R . .  
 H2B H 0.2227 -0.0610 0.7201 0.027 Uiso 1 1 d R . .  
 N3 N 0.3016(2) 0.0934(2) 0.66825(13) 0.0187(8) Uani 1 1 d . . .  
 H3A H 0.2889 0.1565 0.6636 0.028 Uiso 1 1 d R . .  
 H3B H 0.2637 0.0552 0.6476 0.028 Uiso 1 1 d R . .  
 N4 N 0.4091(2) 0.0173(2) 0.74780(14) 0.0191(8) Uani 1 1 d . . .  
 H4A H 0.4646 0.0462 0.7576 0.029 Uiso 1 1 d R . .  
 H4B H 0.4091 -0.0344 0.7702 0.029 Uiso 1 1 d R . .  
 N5 N 0.3480(2) 0.2162(2) 0.75468(14) 0.0195(8) Uani 1 1 d . B .  
 H5A H 0.4127 0.2107 0.7471 0.023 Uiso 1 1 calc R . .  
 H5B H 0.3211 0.2569 0.7291 0.023 Uiso 1 1 calc R . .  
 N6 N 0.2910(2) 0.0946(2) 0.83019(13) 0.0177(8) Uani 1 1 d . . .  
 H6A H 0.2314 0.1055 0.8434 0.027 Uiso 1 1 d R . .  
 H6B H 0.3012 0.0356 0.8445 0.027 Uiso 1 1 d R . .  
 C1 C 0.0856(3) 0.0749(3) 0.72838(16) 0.0172(9) Uani 1 1 d . . .

H1 H 0.0995 0.0540 0.6898 0.021 Uiso 1 1 calc R . . .  
C2 C -0.0144(3) 0.1167(3) 0.72969(18) 0.0231(10) Uani 1 1 d . . .  
C3 C -0.0462(3) 0.1657(3) 0.6834(2) 0.0394(13) Uani 1 1 d . . .  
H3 H -0.0077 0.1663 0.6511 0.047 Uiso 1 1 calc R . . .  
C4 C -0.1339(4) 0.2138(4) 0.6841(3) 0.0617(19) Uani 1 1 d . . .  
H4 H -0.1551 0.2474 0.6523 0.074 Uiso 1 1 calc R . . .  
C5 C -0.1900(4) 0.2129(4) 0.7303(3) 0.0599(19) Uani 1 1 d . . .  
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C6 C -0.1610(3) 0.1631(4) 0.7758(3) 0.0473(15) Uani 1 1 d . . .  
H6 H -0.2010 0.1612 0.8075 0.057 Uiso 1 1 calc R . . .  
C7 C -0.0731(3) 0.1150(3) 0.7757(2) 0.0292(11) Uani 1 1 d . . .  
H7 H -0.0531 0.0806 0.8076 0.035 Uiso 1 1 calc R . . .  
C8 C 0.1090(3) -0.0092(3) 0.76670(15) 0.0144(9) Uani 1 1 d . . .  
H8 H 0.1083 0.0165 0.8051 0.017 Uiso 1 1 calc R . . .  
C9 C 0.0414(3) -0.0938(3) 0.76504(18) 0.0225(10) Uani 1 1 d . . .  
C10 C 0.0094(4) -0.1351(3) 0.8133(2) 0.0400(13) Uani 1 1 d . . .  
H10 H 0.0319 -0.1104 0.8474 0.048 Uiso 1 1 calc R . . .  
C11 C -0.0552(4) -0.2120(4) 0.8134(3) 0.0501(15) Uani 1 1 d . . .  
H11 H -0.0766 -0.2389 0.8472 0.060 Uiso 1 1 calc R . . .  
C12 C -0.0874(4) -0.2486(3) 0.7649(2) 0.0436(14) Uani 1 1 d . . .  
H12 H -0.1314 -0.3010 0.7648 0.052 Uiso 1 1 calc R . . .  
C13 C -0.0559(3) -0.2092(4) 0.7156(2) 0.0388(14) Uani 1 1 d . . .  
H13 H -0.0776 -0.2353 0.6817 0.047 Uiso 1 1 calc R . . .  
C14 C 0.0077(3) -0.1314(3) 0.71602(19) 0.0290(11) Uani 1 1 d . . .  
H14 H 0.0281 -0.1039 0.6822 0.035 Uiso 1 1 calc R . . .  
C15 C 0.4057(3) 0.0717(3) 0.65477(16) 0.0210(10) Uani 1 1 d . . .  
H15 H 0.4454 0.1261 0.6694 0.025 Uiso 1 1 calc R . . .  
C16 C 0.4242(3) 0.0655(3) 0.59361(17) 0.0258(11) Uani 1 1 d . . .  
C17 C 0.4019(3) -0.0141(4) 0.56247(18) 0.0319(12) Uani 1 1 d . . .  
H17 H 0.3760 -0.0696 0.5799 0.038 Uiso 1 1 calc R . . .  
C18 C 0.4165(3) -0.0148(4) 0.5059(2) 0.0413(13) Uani 1 1 d . . .  
H18 H 0.4003 -0.0700 0.4847 0.050 Uiso 1 1 calc R . . .  
C19 C 0.4548(4) 0.0655(5) 0.4811(2) 0.0524(16) Uani 1 1 d . . .  
H19 H 0.4647 0.0660 0.4425 0.063 Uiso 1 1 calc R . . .  
C20 C 0.4787(4) 0.1448(4) 0.5116(2) 0.0520(15) Uani 1 1 d . . .  
H20 H 0.5066 0.1994 0.4942 0.062 Uiso 1 1 calc R . . .  
C21 C 0.4627(4) 0.1461(4) 0.5680(2) 0.0383(13) Uani 1 1 d . . .  
H21 H 0.4780 0.2019 0.5889 0.046 Uiso 1 1 calc R . . .  
C22 C 0.4276(3) -0.0169(3) 0.68999(16) 0.0207(10) Uani 1 1 d . . .  
H22 H 0.3772 -0.0661 0.6813 0.025 Uiso 1 1 calc R . . .  
C23 C 0.5246(3) -0.0651(3) 0.68234(17) 0.0231(10) Uani 1 1 d . . .  
C24 C 0.5284(3) -0.1623(3) 0.66982(18) 0.0314(12) Uani 1 1 d . . .  
H24 H 0.4703 -0.1976 0.6652 0.038 Uiso 1 1 calc R . . .  
C25 C 0.6159(4) -0.2084(4) 0.6641(2) 0.0403(13) Uani 1 1 d . . .  
H25 H 0.6177 -0.2747 0.6544 0.048 Uiso 1 1 calc R . . .  
C26 C 0.6997(4) -0.1595(4) 0.67218(19) 0.0450(15) Uani 1 1 d . . .

H26 H 0.7597 -0.1921 0.6694 0.054 Uiso 1 1 calc R ..  
C27 C 0.6976(3) -0.0621(4) 0.6845(2) 0.0442(14) Uani 1 1 d ...  
H27 H 0.7560 -0.0276 0.6896 0.053 Uiso 1 1 calc R ..  
C28 C 0.6101(3) -0.0154(4) 0.68931(18) 0.0357(13) Uani 1 1 d ...  
H28 H 0.6087 0.0516 0.6975 0.043 Uiso 1 1 calc R ..  
C29 C 0.3350(3) 0.2573(3) 0.81048(16) 0.0182(9) Uani 1 1 d D ..  
H29 H 0.2654 0.2749 0.8145 0.022 Uiso 1 1 calc R A 1  
C30 C 0.3928(3) 0.3475(3) 0.81919(18) 0.0259(11) Uani 0.760(6) 1 d PD B 1  
C31 C 0.3520(5) 0.4347(4) 0.8016(3) 0.0308(19) Uani 0.760(6) 1 d PD B 1  
H31 H 0.2919 0.4357 0.7830 0.037 Uiso 0.760(6) 1 calc PR B 1  
C32 C 0.4025(5) 0.5208(4) 0.8124(3) 0.0406(18) Uani 0.760(6) 1 d PD B 1  
H32 H 0.3780 0.5804 0.7992 0.049 Uiso 0.760(6) 1 calc PR B 1  
C33 C 0.4876(5) 0.5187(4) 0.8422(3) 0.0399(18) Uani 0.760(6) 1 d PD B 1  
H33 H 0.5205 0.5773 0.8496 0.048 Uiso 0.760(6) 1 calc PR B 1  
C34 C 0.5248(5) 0.4340(5) 0.8610(3) 0.035(2) Uani 0.760(6) 1 d PD B 1  
H34 H 0.5811 0.4341 0.8833 0.042 Uiso 0.760(6) 1 calc PR B 1  
C35 C 0.4796(8) 0.3467(8) 0.8475(7) 0.0339(12) Uani 0.760(6) 1 d PD B 1  
H35 H 0.5084 0.2871 0.8577 0.041 Uiso 0.760(6) 1 calc PR B 1  
C30A C 0.3928(3) 0.3475(3) 0.81919(18) 0.0259(11) Uani 0.240(6) 1 d PD B 2  
C31A C 0.3803(14) 0.4289(11) 0.7836(8) 0.0308(19) Uani 0.240(6) 1 d PD B 2  
H31A H 0.3236 0.4311 0.7617 0.037 Uiso 0.240(6) 1 calc PR B 2  
C32A C 0.4465(14) 0.5064(12) 0.7787(8) 0.0406(18) Uani 0.240(6) 1 d PD B 2  
H32A H 0.4333 0.5593 0.7550 0.049 Uiso 0.240(6) 1 calc PR B 2  
C33A C 0.5308(15) 0.5033(14) 0.8093(9) 0.0399(18) Uani 0.240(6) 1 d PD B 2  
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C34A C 0.5482(16) 0.4225(16) 0.8401(10) 0.035(2) Uani 0.240(6) 1 d PD B 2  
H34A H 0.6098 0.4154 0.8567 0.042 Uiso 0.240(6) 1 calc PR B 2  
C35A C 0.480(2) 0.350(2) 0.848(2) 0.0339(12) Uani 0.240(6) 1 d PD B 2  
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C36 C 0.3551(3) 0.1731(3) 0.84975(17) 0.0207(10) Uani 1 1 d . B .  
H36 H 0.4235 0.1522 0.8445 0.025 Uiso 1 1 calc R ..  
C37 C 0.3397(3) 0.1943(3) 0.91018(16) 0.0181(9) Uani 1 1 d ...  
C38 C 0.2892(3) 0.2733(3) 0.92895(17) 0.0246(10) Uani 1 1 d . B .  
H38 H 0.2651 0.3186 0.9031 0.029 Uiso 1 1 calc R ..  
C39 C 0.2726(3) 0.2884(3) 0.98393(18) 0.0294(11) Uani 1 1 d ...  
H39 H 0.2387 0.3440 0.9960 0.035 Uiso 1 1 calc R B .  
C40 C 0.3059(3) 0.2218(4) 1.02140(18) 0.0334(12) Uani 1 1 d . B .  
H40 H 0.2917 0.2294 1.0594 0.040 Uiso 1 1 calc R ..  
C41 C 0.3596(3) 0.1442(3) 1.00386(19) 0.0340(12) Uani 1 1 d ...  
H41 H 0.3850 0.1002 1.0301 0.041 Uiso 1 1 calc R B .  
C42 C 0.3772(3) 0.1296(3) 0.94820(18) 0.0282(11) Uani 1 1 d . B .  
H42 H 0.4144 0.0760 0.9363 0.034 Uiso 1 1 calc R ..  
C11 Cl 0.18748(7) -0.08903(7) 0.62064(4) 0.0231(2) Uani 1 1 d ...  
C12 Cl 0.22365(8) 0.31487(7) 0.65873(4) 0.0289(3) Uani 1 1 d ...  
C13 Cl 0.37026(7) -0.12578(7) 0.84827(4) 0.0264(2) Uani 1 1 d ...  
O50 O 0.5875(2) 0.1026(2) 0.81981(12) 0.0321(8) Uani 1 1 d ...

H50 H 0.6084 0.1437 0.8422 0.048 Uiso 1 1 calc R . .  
 C51 C 0.6295(4) 0.0117(3) 0.8314(2) 0.0415(13) Uani 1 1 d . . .  
 H51A H 0.6874 0.0031 0.8088 0.062 Uiso 1 1 calc R . .  
 H51B H 0.5831 -0.0395 0.8230 0.062 Uiso 1 1 calc R . .  
 H51C H 0.6471 0.0087 0.8704 0.062 Uiso 1 1 calc R . .  
 O55 O 0.6260(3) 0.3787(3) 0.68996(18) 0.0612(11) Uani 0.88 1 d P . .  
 H55 H 0.6699 0.3925 0.6669 0.092 Uiso 0.88 1 d PR . .  
 C56 C 0.5991(5) 0.4608(5) 0.7179(3) 0.0612(11) Uani 0.88 1 d P . .  
 H56A H 0.5912 0.5140 0.6919 0.092 Uiso 0.88 1 calc PR . .  
 H56B H 0.6489 0.4774 0.7449 0.092 Uiso 0.88 1 calc PR . .  
 H56C H 0.5379 0.4492 0.7370 0.092 Uiso 0.88 1 calc PR . .  
 O60 O 0.5691(2) -0.2372(2) 0.86368(13) 0.0398(8) Uani 1 1 d D . .  
 H60 H 0.5160 -0.2074 0.8596 0.060 Uiso 1 1 d RD . .  
 C61 C 0.6065(4) -0.2474(4) 0.8101(2) 0.0577(17) Uani 1 1 d . . .  
 H61A H 0.5607 -0.2837 0.7875 0.087 Uiso 1 1 calc R . .  
 H61B H 0.6679 -0.2822 0.8117 0.087 Uiso 1 1 calc R . .  
 H61C H 0.6168 -0.1835 0.7940 0.087 Uiso 1 1 calc R . .  
 O65 O 0.5495(2) 0.2139(2) 0.72757(13) 0.0374(8) Uani 1 1 d . . .  
 H65A H 0.5730 0.2000 0.7588 0.056 Uiso 1 1 d R . .  
 H65B H 0.5731 0.2669 0.7165 0.056 Uiso 1 1 d R . .

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 N2 0.0135(17) 0.0181(18) 0.022(2) 0.0007(15) 0.0009(15) 0.0028(15)  
 N3 0.0163(18) 0.025(2) 0.015(2) -0.0010(15) 0.0010(14) -0.0007(16)  
 N4 0.0148(17) 0.0241(19) 0.019(2) -0.0002(15) -0.0024(15) 0.0028(15)  
 N5 0.0168(17) 0.0277(19) 0.014(2) 0.0008(16) -0.0021(15) 0.0030(16)  
 N6 0.0171(19) 0.0175(19) 0.019(2) 0.0019(14) -0.0026(14) 0.0023(16)  
 C1 0.014(2) 0.019(2) 0.018(2) -0.0039(17) 0.0000(17) -0.0017(19)  
 C2 0.017(2) 0.019(2) 0.034(3) -0.0058(19) -0.007(2) 0.004(2)  
 C3 0.019(3) 0.038(3) 0.061(4) 0.022(3) -0.003(2) -0.003(2)  
 C4 0.019(3) 0.053(4) 0.113(6) 0.045(4) -0.008(3) 0.002(3)  
 C5 0.012(3) 0.030(3) 0.137(7) 0.012(4) -0.005(3) 0.004(3)  
 C6 0.027(3) 0.031(3) 0.084(5) -0.019(3) 0.010(3) -0.002(3)  
 C7 0.014(2) 0.035(3) 0.039(3) -0.008(2) 0.001(2) -0.004(2)  
 C8 0.012(2) 0.019(2) 0.012(2) -0.0004(16) -0.0024(16) 0.0046(19)  
 C9 0.020(2) 0.017(2) 0.031(3) -0.0021(19) -0.0047(19) 0.000(2)  
 C10 0.045(3) 0.040(3) 0.035(3) 0.011(2) -0.008(2) -0.015(3)

C11 0.043(3) 0.044(3) 0.063(4) 0.020(3) -0.007(3) -0.020(3)  
 C12 0.033(3) 0.026(3) 0.072(5) 0.002(3) -0.007(3) -0.011(2)  
 C13 0.016(3) 0.037(3) 0.064(4) -0.027(3) -0.007(2) -0.001(2)  
 C14 0.020(2) 0.028(3) 0.039(3) -0.011(2) 0.005(2) 0.005(2)  
 C15 0.012(2) 0.034(3) 0.017(3) 0.0004(19) 0.0003(18) 0.001(2)  
 C16 0.016(2) 0.044(3) 0.017(3) 0.005(2) 0.0034(19) 0.015(2)  
 C17 0.024(3) 0.051(3) 0.020(3) -0.002(2) 0.003(2) 0.002(2)  
 C18 0.034(3) 0.068(4) 0.021(3) -0.010(3) -0.003(2) 0.013(3)  
 C19 0.060(4) 0.081(5) 0.016(3) 0.015(3) 0.004(2) 0.026(4)  
 C20 0.068(4) 0.046(3) 0.042(4) 0.011(3) 0.021(3) 0.011(3)  
 C21 0.050(3) 0.044(3) 0.020(3) 0.011(2) 0.013(2) 0.014(3)  
 C22 0.020(2) 0.034(3) 0.008(2) 0.0007(18) -0.0041(17) 0.007(2)  
 C23 0.019(2) 0.037(3) 0.013(2) -0.0017(19) 0.0035(18) 0.010(2)  
 C24 0.023(3) 0.047(3) 0.024(3) -0.003(2) -0.002(2) 0.008(2)  
 C25 0.035(3) 0.050(3) 0.036(3) -0.002(2) -0.003(2) 0.016(3)  
 C26 0.038(3) 0.077(4) 0.020(3) 0.001(3) 0.003(2) 0.038(3)  
 C27 0.015(3) 0.085(5) 0.032(3) 0.001(3) 0.000(2) 0.009(3)  
 C28 0.021(3) 0.058(3) 0.028(3) -0.004(2) 0.006(2) 0.003(3)  
 C29 0.016(2) 0.019(2) 0.020(3) 0.0018(17) -0.0049(18) -0.001(2)  
 C30 0.026(3) 0.018(2) 0.034(3) -0.003(2) -0.009(2) -0.001(2)  
 C31 0.022(4) 0.024(3) 0.047(5) 0.006(3) -0.006(3) -0.002(3)  
 C32 0.054(5) 0.022(3) 0.045(5) 0.012(3) -0.005(3) 0.010(3)  
 C33 0.055(5) 0.023(3) 0.042(5) 0.002(3) -0.014(4) -0.017(3)  
 C34 0.038(4) 0.036(4) 0.031(5) 0.001(4) -0.014(3) -0.014(3)  
 C35 0.043(3) 0.021(3) 0.037(3) 0.005(2) -0.018(2) -0.007(2)  
 C30A 0.026(3) 0.018(2) 0.034(3) -0.003(2) -0.009(2) -0.001(2)  
 C31A 0.022(4) 0.024(3) 0.047(5) 0.006(3) -0.006(3) -0.002(3)  
 C32A 0.054(5) 0.022(3) 0.045(5) 0.012(3) -0.005(3) 0.010(3)  
 C33A 0.055(5) 0.023(3) 0.042(5) 0.002(3) -0.014(4) -0.017(3)  
 C34A 0.038(4) 0.036(4) 0.031(5) 0.001(4) -0.014(3) -0.014(3)  
 C35A 0.043(3) 0.021(3) 0.037(3) 0.005(2) -0.018(2) -0.007(2)  
 C36 0.017(2) 0.021(2) 0.025(3) -0.0001(19) -0.0045(18) 0.003(2)  
 C37 0.016(2) 0.023(2) 0.015(2) -0.0020(19) -0.0048(18) -0.002(2)  
 C38 0.030(3) 0.029(3) 0.014(3) -0.0059(19) -0.0091(19) -0.001(2)  
 C39 0.025(3) 0.036(3) 0.028(3) -0.007(2) -0.004(2) 0.001(2)  
 C40 0.035(3) 0.050(3) 0.016(3) -0.006(2) 0.000(2) -0.010(3)  
 C41 0.038(3) 0.041(3) 0.023(3) 0.011(2) -0.007(2) -0.007(2)  
 C42 0.032(3) 0.029(3) 0.023(3) 0.000(2) -0.003(2) 0.006(2)  
 CI1 0.0304(6) 0.0201(5) 0.0186(6) -0.0016(4) 0.0001(4) -0.0041(5)  
 CI2 0.0319(6) 0.0266(6) 0.0283(6) 0.0093(5) -0.0040(5) -0.0022(5)  
 CI3 0.0313(6) 0.0272(6) 0.0206(6) 0.0014(5) -0.0020(5) 0.0054(5)  
 O50 0.0319(18) 0.0340(19) 0.030(2) -0.0011(15) -0.0075(14) 0.0003(16)  
 C51 0.052(3) 0.036(3) 0.037(3) 0.004(2) -0.012(2) -0.005(3)  
 O55 0.046(2) 0.066(3) 0.072(3) 0.013(2) 0.0157(19) 0.003(2)  
 C56 0.046(2) 0.066(3) 0.072(3) 0.013(2) 0.0157(19) 0.003(2)  
 O60 0.043(2) 0.039(2) 0.037(2) 0.0011(15) -0.0046(16) 0.0095(17)

C61 0.076(4) 0.051(4) 0.046(4) -0.010(3) 0.019(3) -0.002(3)  
O65 0.0221(17) 0.051(2) 0.039(2) 0.0042(16) -0.0028(14) -0.0075(16)

\_geom\_special\_details

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All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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loop\_

\_geom\_bond\_atom\_site\_label\_1  
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\_geom\_bond\_distance  
\_geom\_bond\_site\_symmetry\_2  
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Co1 N5 1.957(3) . ?

Co1 N6 1.962(3) . ?

Co1 N4 1.967(3) . ?

Co1 N1 1.970(3) . ?

Co1 N2 1.989(3) . ?

Co1 N3 1.989(3) . ?

N1 C1 1.504(5) . ?

N1 H1A 0.9000 . ?

N1 H1B 0.9000 . ?

N2 C8 1.504(4) . ?

N2 H2A 0.8998 . ?

N2 H2B 0.9003 . ?

N3 C15 1.512(5) . ?

N3 H3A 0.8999 . ?

N3 H3B 0.9000 . ?

N4 C22 1.506(5) . ?

N4 H4A 0.9001 . ?

N4 H4B 0.8999 . ?

N5 C29 1.483(5) . ?

N5 H5A 0.9200 . ?

N5 H5B 0.9200 . ?

N6 C36 1.485(5) . ?

N6 H6A 0.9003 . ?

N6 H6B 0.9001 . ?

C1 C2 1.504(5) . ?

C1 C8 1.528(5) . ?

C1 H1 1.0000 . ?

C2 C7 1.385(6) . ?  
C2 C3 1.387(6) . ?  
C3 C4 1.388(7) . ?  
C3 H3 0.9500 . ?  
C4 C5 1.365(8) . ?  
C4 H4 0.9500 . ?  
C5 C6 1.366(8) . ?  
C5 H5 0.9500 . ?  
C6 C7 1.390(6) . ?  
C6 H6 0.9500 . ?  
C7 H7 0.9500 . ?  
C8 C9 1.504(5) . ?  
C8 H8 1.0000 . ?  
C9 C10 1.380(6) . ?  
C9 C14 1.383(6) . ?  
C10 C11 1.393(7) . ?  
C10 H10 0.9500 . ?  
C11 C12 1.358(7) . ?  
C11 H11 0.9500 . ?  
C12 C13 1.388(7) . ?  
C12 H12 0.9500 . ?  
C13 C14 1.394(6) . ?  
C13 H13 0.9500 . ?  
C14 H14 0.9500 . ?  
C15 C16 1.512(6) . ?  
C15 C22 1.527(6) . ?  
C15 H15 1.0000 . ?  
C16 C17 1.374(6) . ?  
C16 C21 1.387(6) . ?  
C17 C18 1.392(6) . ?  
C17 H17 0.9500 . ?  
C18 C19 1.372(7) . ?  
C18 H18 0.9500 . ?  
C19 C20 1.368(8) . ?  
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C23 C24 1.383(6) . ?  
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C25 H25 0.9500 . ?

C26 C27 1.384(7) . ?  
C26 H26 0.9500 . ?  
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C28 H28 0.9500 . ?  
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C29 C36 1.535(5) . ?  
C29 H29 1.0000 . ?  
C30 C35 1.387(7) . ?  
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C35 H35 0.9500 . ?  
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C36 C37 1.514(6) . ?  
C36 H36 1.0000 . ?  
C37 C38 1.379(6) . ?  
C37 C42 1.389(6) . ?  
C38 C39 1.373(6) . ?  
C38 H38 0.9500 . ?  
C39 C40 1.377(6) . ?  
C39 H39 0.9500 . ?  
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C40 H40 0.9500 . ?  
C41 C42 1.390(6) . ?  
C41 H41 0.9500 . ?  
C42 H42 0.9500 . ?  
O50 C51 1.418(5) . ?  
O50 H50 0.8400 . ?  
C51 H51A 0.9800 . ?  
C51 H51B 0.9800 . ?  
C51 H51C 0.9800 . ?

O55 C56 1.378(7) . ?  
O55 H55 0.8502 . ?  
C56 H56A 0.9800 . ?  
C56 H56B 0.9800 . ?  
C56 H56C 0.9800 . ?  
O60 C61 1.409(6) . ?  
O60 H60 0.8499 . ?  
C61 H61A 0.9800 . ?  
C61 H61B 0.9800 . ?  
C61 H61C 0.9800 . ?  
O65 H65A 0.8495 . ?  
O65 H65B 0.8493 . ?

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N4 Co1 N1 172.66(14) . . ?  
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N6 Co1 N2 90.37(14) . . ?  
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N6 Co1 N3 171.66(13) . . ?  
N4 Co1 N3 84.56(13) . . ?  
N1 Co1 N3 90.74(13) . . ?  
N2 Co1 N3 96.72(14) . . ?  
C1 N1 Co1 109.4(2) . . ?  
C1 N1 H1A 107.3 . . ?  
Co1 N1 H1A 115.2 . . ?  
C1 N1 H1B 106.9 . . ?  
Co1 N1 H1B 115.3 . . ?  
H1A N1 H1B 101.9 . . ?  
C8 N2 Co1 108.8(2) . . ?  
C8 N2 H2A 107.5 . . ?  
Co1 N2 H2A 112.1 . . ?  
C8 N2 H2B 116.6 . . ?

Co1 N2 H2B 104.5 . . ?  
H2A N2 H2B 107.5 . . ?  
C15 N3 Co1 107.9(2) . . ?  
C15 N3 H3A 110.7 . . ?  
Co1 N3 H3A 97.7 . . ?  
C15 N3 H3B 108.6 . . ?  
Co1 N3 H3B 118.7 . . ?  
H3A N3 H3B 112.8 . . ?  
C22 N4 Co1 109.1(2) . . ?  
C22 N4 H4A 104.0 . . ?  
Co1 N4 H4A 120.2 . . ?  
C22 N4 H4B 108.3 . . ?  
Co1 N4 H4B 113.1 . . ?  
H4A N4 H4B 101.2 . . ?  
C29 N5 Co1 110.6(2) . . ?  
C29 N5 H5A 109.5 . . ?  
Co1 N5 H5A 109.5 . . ?  
C29 N5 H5B 109.5 . . ?  
Co1 N5 H5B 109.5 . . ?  
H5A N5 H5B 108.1 . . ?  
C36 N6 Co1 111.4(2) . . ?  
C36 N6 H6A 108.2 . . ?  
Co1 N6 H6A 109.6 . . ?  
C36 N6 H6B 116.7 . . ?  
Co1 N6 H6B 110.9 . . ?  
H6A N6 H6B 99.2 . . ?  
C2 C1 N1 110.6(3) . . ?  
C2 C1 C8 118.5(3) . . ?  
N1 C1 C8 103.2(3) . . ?  
C2 C1 H1 108.0 . . ?  
N1 C1 H1 108.0 . . ?  
C8 C1 H1 108.0 . . ?  
C7 C2 C3 118.6(4) . . ?  
C7 C2 C1 123.6(4) . . ?  
C3 C2 C1 117.7(4) . . ?  
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C6 C5 H5 119.9 . . ?  
C5 C6 C7 120.0(5) . . ?  
C5 C6 H6 120.0 . . ?

C7 C6 H6 120.0 . . ?  
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N2 C8 C1 103.4(3) . . ?  
C9 C8 C1 116.6(3) . . ?  
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C1 C8 H8 107.2 . . ?  
C10 C9 C14 117.9(4) . . ?  
C10 C9 C8 120.1(4) . . ?  
C14 C9 C8 121.9(4) . . ?  
C9 C10 C11 121.7(5) . . ?  
C9 C10 H10 119.1 . . ?  
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C11 C12 C13 120.0(5) . . ?  
C11 C12 H12 120.0 . . ?  
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C9 C14 H14 119.6 . . ?  
C13 C14 H14 119.6 . . ?  
C16 C15 N3 112.7(3) . . ?  
C16 C15 C22 118.2(3) . . ?  
N3 C15 C22 103.2(3) . . ?  
C16 C15 H15 107.4 . . ?  
N3 C15 H15 107.4 . . ?  
C22 C15 H15 107.4 . . ?  
C17 C16 C21 119.1(4) . . ?  
C17 C16 C15 123.3(4) . . ?  
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C18 C19 H19 119.7 . . ?

C19 C20 C21 120.4(5) . . ?  
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C16 C21 C20 119.7(5) . . ?  
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C20 C21 H21 120.1 . . ?  
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N4 C22 C15 103.7(3) . . ?  
C23 C22 C15 117.6(3) . . ?  
N4 C22 H22 107.0 . . ?  
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C15 C22 H22 107.0 . . ?  
C28 C23 C24 118.7(4) . . ?  
C28 C23 C22 121.8(4) . . ?  
C24 C23 C22 119.4(4) . . ?  
C25 C24 C23 120.5(4) . . ?  
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C23 C24 H24 119.8 . . ?  
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C24 C25 H25 119.8 . . ?  
C25 C26 C27 120.0(5) . . ?  
C25 C26 H26 120.0 . . ?  
C27 C26 H26 120.0 . . ?  
C28 C27 C26 119.7(5) . . ?  
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C27 C28 H28 119.7 . . ?  
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N5 C29 C30 112.6(3) . . ?  
N5 C29 C36 104.7(3) . . ?  
C30 C29 C36 116.7(3) . . ?  
N5 C29 H29 107.5 . . ?  
C30 C29 H29 107.5 . . ?  
C36 C29 H29 107.5 . . ?  
C35 C30 C31 120.6(6) . . ?  
C35 C30 C29 121.9(5) . . ?  
C31 C30 C29 117.4(4) . . ?  
C30 C31 C32 118.3(5) . . ?  
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C34 C33 C32 121.1(6) . . ?

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C33 C34 H34 120.1 . . ?  
C35 C34 H34 120.1 . . ?  
C30 C35 C34 119.8(8) . . ?  
C30 C35 H35 120.1 . . ?  
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C33A C32A C31A 118.5(15) . . ?  
C33A C32A H32A 120.8 . . ?  
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C34A C33A C32A 117.9(16) . . ?  
C34A C33A H33A 121.0 . . ?  
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C33A C34A H34A 118.4 . . ?  
C35A C34A H34A 118.4 . . ?  
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N6 C36 C37 111.6(3) . . ?  
N6 C36 C29 104.5(3) . . ?  
C37 C36 C29 115.5(3) . . ?  
N6 C36 H36 108.3 . . ?  
C37 C36 H36 108.3 . . ?  
C29 C36 H36 108.3 . . ?  
C38 C37 C42 118.9(4) . . ?  
C38 C37 C36 123.2(4) . . ?  
C42 C37 C36 117.9(4) . . ?  
C39 C38 C37 121.9(4) . . ?  
C39 C38 H38 119.0 . . ?  
C37 C38 H38 119.0 . . ?  
C38 C39 C40 119.1(4) . . ?  
C38 C39 H39 120.5 . . ?  
C40 C39 H39 120.5 . . ?  
C41 C40 C39 120.1(4) . . ?  
C41 C40 H40 120.0 . . ?  
C39 C40 H40 120.0 . . ?  
C40 C41 C42 120.7(4) . . ?  
C40 C41 H41 119.6 . . ?  
C42 C41 H41 119.6 . . ?  
C37 C42 C41 119.2(4) . . ?  
C37 C42 H42 120.4 . . ?  
C41 C42 H42 120.4 . . ?  
C51 O50 H50 109.5 . . ?  
O50 C51 H51A 109.5 . . ?  
O50 C51 H51B 109.5 . . ?

H51A C51 H51B 109.5 . . ?  
O50 C51 H51C 109.5 . . ?  
H51A C51 H51C 109.5 . . ?  
H51B C51 H51C 109.5 . . ?  
C56 O55 H55 109.5 . . ?  
O55 C56 H56A 109.5 . . ?  
O55 C56 H56B 109.5 . . ?  
H56A C56 H56B 109.5 . . ?  
O55 C56 H56C 109.5 . . ?  
H56A C56 H56C 109.5 . . ?  
H56B C56 H56C 109.5 . . ?  
C61 O60 H60 105.1 . . ?  
O60 C61 H61A 109.5 . . ?  
O60 C61 H61B 109.5 . . ?  
H61A C61 H61B 109.5 . . ?  
O60 C61 H61C 109.5 . . ?  
H61A C61 H61C 109.5 . . ?  
H61B C61 H61C 109.5 . . ?  
H65A O65 H65B 109.5 . . ?

loop\_  
  \_geom\_torsion\_atom\_site\_label\_1  
  \_geom\_torsion\_atom\_site\_label\_2  
  \_geom\_torsion\_atom\_site\_label\_3  
  \_geom\_torsion\_atom\_site\_label\_4  
  \_geom\_torsion  
  \_geom\_torsion\_site\_symmetry\_1  
  \_geom\_torsion\_site\_symmetry\_2  
  \_geom\_torsion\_site\_symmetry\_3  
  \_geom\_torsion\_site\_symmetry\_4  
  \_geom\_torsion\_publ\_flag  
N5 Co1 N1 C1 169.2(3) . . . . ?  
N6 Co1 N1 C1 -107.0(2) . . . . ?  
N4 Co1 N1 C1 29.6(13) . . . . ?  
N2 Co1 N1 C1 -17.1(3) . . . . ?  
N3 Co1 N1 C1 79.6(3) . . . . ?  
N5 Co1 N2 C8 32.0(11) . . . . ?  
N6 Co1 N2 C8 77.4(2) . . . . ?  
N4 Co1 N2 C8 168.4(2) . . . . ?  
N1 Co1 N2 C8 -17.0(2) . . . . ?  
N3 Co1 N2 C8 -107.0(2) . . . . ?  
N5 Co1 N3 C15 76.8(2) . . . . ?  
N6 Co1 N3 C15 39.4(10) . . . . ?  
N4 Co1 N3 C15 -18.3(2) . . . . ?  
N1 Co1 N3 C15 167.4(2) . . . . ?  
N2 Co1 N3 C15 -108.7(2) . . . . ?

N5 Co1 N4 C22 -104.8(3) . . . ?  
N6 Co1 N4 C22 171.4(3) . . . ?  
N1 Co1 N4 C22 34.7(13) . . . ?  
N2 Co1 N4 C22 81.0(3) . . . ?  
N3 Co1 N4 C22 -15.6(3) . . . ?  
N6 Co1 N5 C29 -17.7(2) . . . ?  
N4 Co1 N5 C29 -108.1(2) . . . ?  
N1 Co1 N5 C29 76.7(3) . . . ?  
N2 Co1 N5 C29 28.0(11) . . . ?  
N3 Co1 N5 C29 167.4(2) . . . ?  
N5 Co1 N6 C36 -13.6(2) . . . ?  
N4 Co1 N6 C36 81.3(3) . . . ?  
N1 Co1 N6 C36 -103.8(2) . . . ?  
N2 Co1 N6 C36 172.3(2) . . . ?  
N3 Co1 N6 C36 24.0(11) . . . ?  
Co1 N1 C1 C2 174.1(3) . . . ?  
Co1 N1 C1 C8 46.4(3) . . . ?  
N1 C1 C2 C7 -90.7(5) . . . ?  
C8 C1 C2 C7 28.1(6) . . . ?  
N1 C1 C2 C3 84.5(5) . . . ?  
C8 C1 C2 C3 -156.7(4) . . . ?  
C7 C2 C3 C4 1.7(7) . . . ?  
C1 C2 C3 C4 -173.8(4) . . . ?  
C2 C3 C4 C5 -0.3(8) . . . ?  
C3 C4 C5 C6 -1.3(9) . . . ?  
C4 C5 C6 C7 1.6(8) . . . ?  
C3 C2 C7 C6 -1.3(6) . . . ?  
C1 C2 C7 C6 173.8(4) . . . ?  
C5 C6 C7 C2 -0.3(7) . . . ?  
Co1 N2 C8 C9 174.2(3) . . . ?  
Co1 N2 C8 C1 46.2(3) . . . ?  
C2 C1 C8 N2 178.5(3) . . . ?  
N1 C1 C8 N2 -59.0(3) . . . ?  
C2 C1 C8 C9 51.7(5) . . . ?  
N1 C1 C8 C9 174.2(3) . . . ?  
N2 C8 C9 C10 104.5(5) . . . ?  
C1 C8 C9 C10 -134.6(4) . . . ?  
N2 C8 C9 C14 -76.9(5) . . . ?  
C1 C8 C9 C14 44.0(5) . . . ?  
C14 C9 C10 C11 -0.3(7) . . . ?  
C8 C9 C10 C11 178.4(4) . . . ?  
C9 C10 C11 C12 0.6(8) . . . ?  
C10 C11 C12 C13 0.0(8) . . . ?  
C11 C12 C13 C14 -0.9(7) . . . ?  
C10 C9 C14 C13 -0.6(6) . . . ?  
C8 C9 C14 C13 -179.3(4) . . . ?

C12 C13 C14 C9 1.2(7) . . . ?  
Co1 N3 C15 C16 175.8(3) . . . ?  
Co1 N3 C15 C22 47.1(3) . . . ?  
N3 C15 C16 C17 -79.0(5) . . . ?  
C22 C15 C16 C17 41.4(6) . . . ?  
N3 C15 C16 C21 98.9(4) . . . ?  
C22 C15 C16 C21 -140.7(4) . . . ?  
C21 C16 C17 C18 -0.6(6) . . . ?  
C15 C16 C17 C18 177.3(4) . . . ?  
C16 C17 C18 C19 0.6(7) . . . ?  
C17 C18 C19 C20 0.4(7) . . . ?  
C18 C19 C20 C21 -1.5(8) . . . ?  
C17 C16 C21 C20 -0.5(7) . . . ?  
C15 C16 C21 C20 -178.5(4) . . . ?  
C19 C20 C21 C16 1.5(8) . . . ?  
Co1 N4 C22 C23 174.4(3) . . . ?  
Co1 N4 C22 C15 45.4(3) . . . ?  
C16 C15 C22 N4 175.5(3) . . . ?  
N3 C15 C22 N4 -59.3(4) . . . ?  
C16 C15 C22 C23 48.8(5) . . . ?  
N3 C15 C22 C23 174.0(3) . . . ?  
N4 C22 C23 C28 -64.2(5) . . . ?  
C15 C22 C23 C28 57.4(5) . . . ?  
N4 C22 C23 C24 113.6(4) . . . ?  
C15 C22 C23 C24 -124.8(4) . . . ?  
C28 C23 C24 C25 -0.4(7) . . . ?  
C22 C23 C24 C25 -178.3(4) . . . ?  
C23 C24 C25 C26 1.9(7) . . . ?  
C24 C25 C26 C27 -2.2(7) . . . ?  
C25 C26 C27 C28 1.0(7) . . . ?  
C26 C27 C28 C23 0.5(7) . . . ?  
C24 C23 C28 C27 -0.7(6) . . . ?  
C22 C23 C28 C27 177.1(4) . . . ?  
Co1 N5 C29 C30 171.3(3) . . . ?  
Co1 N5 C29 C36 43.5(3) . . . ?  
N5 C29 C30 C35 -100.5(10) . . . ?  
C36 C29 C30 C35 20.7(11) . . . ?  
N5 C29 C30 C31 84.8(5) . . . ?  
C36 C29 C30 C31 -154.0(4) . . . ?  
C35 C30 C31 C32 1.4(11) . . . ?  
C29 C30 C31 C32 176.2(5) . . . ?  
C30 C31 C32 C33 -3.4(9) . . . ?  
C31 C32 C33 C34 0.8(10) . . . ?  
C32 C33 C34 C35 3.8(14) . . . ?  
C31 C30 C35 C34 3.1(19) . . . ?  
C29 C30 C35 C34 -171.5(9) . . . ?

C33 C34 C35 C30 -5.7(19) . . . ?  
C31A C32A C33A C34A 4(3) . . . ?  
C32A C33A C34A C35A -9(4) . . . ?  
Co1 N6 C36 C37 165.6(3) . . . ?  
Co1 N6 C36 C29 40.1(3) . . . ?  
N5 C29 C36 N6 -52.8(4) . . . ?  
C30 C29 C36 N6 -178.0(3) . . . ?  
N5 C29 C36 C37 -175.8(3) . . . ?  
C30 C29 C36 C37 58.9(5) . . . ?  
N6 C36 C37 C38 -103.6(4) . . . ?  
C29 C36 C37 C38 15.6(6) . . . ?  
N6 C36 C37 C42 75.2(4) . . . ?  
C29 C36 C37 C42 -165.6(4) . . . ?  
C42 C37 C38 C39 -1.8(6) . . . ?  
C36 C37 C38 C39 177.1(4) . . . ?  
C37 C38 C39 C40 -1.3(6) . . . ?  
C38 C39 C40 C41 3.7(7) . . . ?  
C39 C40 C41 C42 -3.0(7) . . . ?  
C38 C37 C42 C41 2.5(6) . . . ?  
C36 C37 C42 C41 -176.5(4) . . . ?  
C40 C41 C42 C37 -0.1(7) . . . ?

\_diffrn\_measured\_fraction\_theta\_max 0.985  
\_diffrn\_reflns\_theta\_full 60.00  
\_diffrn\_measured\_fraction\_theta\_full 0.985  
\_refine\_diff\_density\_max 0.362  
\_refine\_diff\_density\_min -0.622  
\_refine\_diff\_density\_rms 0.051